



XXXIX Bienal de la Real Sociedad de Física

DONOSTIA - SAN SEBASTIÁN 15-19
Julio 2024

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Programme / Programa

	15 July Monday	16 July Tuesday	17 July Wednesday	18 July Thursday	19 July Friday
	MUSIKENE				
8:30-9:30	REGISTRATION				
8:30-9:00		REGISTRATION	REGISTRATION SCHOOL OF ENGINEERING		
9:30-9:45	WELCOME				
9:00-9:45		Sayeef Salahuddin	Jonathan Home	José Luis Sánchez Gómez	Roberto Gómez Calvet
9:45-10:30	Juan Ignacio Cirac	Ursulla Keller	Jorge Mira	Yolanda Prezado	Alessandra Buonanno
10:30-11:00	COFFEE BREAK				COFFEE BREAK / VOTACIONES
11:00-11:45	Clivia Sotomayor Torres	Francisco Savall	Olga Smirnova	Jorge Méndez	Javier Aizpurua
11:45-13:00	Dialogue 1 The Quantum revolution in the XXI Century	Dialogue 2 Women's leadership in Physics	Dialogue 3 Role of physicist in the XXI century	Dialogue 4 The Impact of Artificial Intelligence on the Physics of the XXI century	ASAMBLEA GENERAL 11:45-12:00 Entrega de premios a las mejores Tesis RSEF-EPJ 12:00-13:00 Junta General Ordinaria RSEF
13:00-14:30	Free time for lunch				Farewell brunch
	SCHOOL OF ENGINEERING OF GIPUZKOA				
14:30-16:00	Symposia 1	Symposia 2	Symposia 3	Symposia 4	
16:00-17:00	COFFEE BREAK AND POSTER SESSION				
17:00-18:30	Symposia 1	Symposia 2	Symposia 3	Symposia 4	
19:00-21:00		DIVULGACIÓN CIENTÍFICA Boulevard de San Sebastián			
20:00	WELCOME RECEPTION Ayuntamiento de San Sebastián *limited capacity. Prior registration is required.		CONFERENCE DINNER Petritegi Departure from Carlos Santamaria Center		

Plenary speakers / Ponentes plenarios



Sayeef Salahuddin

University of California Berkeley, USA

S. Salahuddin is the TSMC Distinguished Professor of Electrical Engineering and Computer Sciences at the University of California Berkeley. His group explores physics for low power electronic and spintronic devices. He is mostly known for the discovery of the Negative Capacitance effect that shows substantial promise for logic, memory and energy storage devices. Salahuddin received the Presidential Early Career Award for Scientist and Engineers (PECASE) from President Obama. Salahuddin also received several other awards including the National Science Foundation CAREER award, the IEEE Nanotechnology Early Career Award, the Young Investigator Awards from the Airforce Office of Scientific Research and the Army Research Office, and the IEEE George E Smith Award. Salahuddin is a co-director of the Berkeley Device Modeling Center (BDMC) and Berkeley Center for Negative Capacitance Transistors (BCNCT). Salahuddin was also a co-director of ASCENT, which is a flagship device technology effort in the US, jointly supported by SRC and DARPA. He served as the chair the IEEE Electron Devices Society committee on Nanotechnology (2014-16) and is currently the Editor-in-Chief of the IEEE Electron Devices Letters, the premier journal for electron devices. Salahuddin is a Fellow of the IEEE and the APS.



Clivia Sotomayor Torres

Director General of the International Iberian Nanotechnology Laboratory (INL) in Braga, Portugal.

Prof. Dr. Clivia. M Sotomayor Torres obtained her PhD in Physics in 1984 from the University of Manchester, UK. She held tenured academic appointments at Saint Andrews and Glasgow universities in the UK, a C4 professorship at Wuppertal University in Germany and was a research professor at the National university of Ireland University College Cork (Tyndall National Institute). From 2007 to 2023 she was an ICREA research professor and group leader of the Phononic and Photonic Nanostructures group at the Catalan Institute of Nanoscience and Nanotechnology in Spain. Clivia received awards from the Royal Society of Edinburgh, the Nuffield Foundation and an Amelia Earhart Fellowship from ZONTA International (USA). She carries out research in the science and engineering of phononic nanostructures, nanophotonics and thermal transport. She was a guest professor at the P. Sabatier Univ. Toulouse, at the Royal Institute of Technology (KTH) in Sweden and the Mittlesten-Scheid Guest Professor at the University of Wuppertal in Germany.

She has supervised over 20 PhD theses and more than 60 postdoctoral researchers. She has published extensively and has been cited over 12 000 times. Since 1989 Clivia has been, and still is, an active participant in European level research and has coordinated several projects. She has held several commissions of trust including membership of the Danish National Research Council board, vice-chair of the Scientific Board of the Silicon Austria Laboratory and co-Chair and Chair of the Advisory Group of the EU Future and Emerging Technologies. In 2020 she was elected to the Academia Europaea and since 2021 she is a holder of an ERC Advanced Grant carrying out research on phonons for information and communication Technologies.

Since September 2023 she is the Director General of the International Iberian Nanotechnology Laboratory (INL) in Braga, Portugal.



Ursula Keller

Professor of Physics at ETH Zurich, Switzerland

Ursula Keller, a tenured physics professor at ETH Zurich since 1993, directed the NCCR MUST ultrafast science program from 2010 to 2022. She earned her Diplom from ETH Zurich in 1984 and a Ph.D. from Stanford University in 1989. As a Member of Technical Staff (MTS) at Bell Labs from 1989 to 1993, she launched her independent research career. Keller co-founded Time-Bandwidth Products (was acquired by JDSU in 2014), and K2 Photonics in 2023. Since 2022, she has served on the supervisory board of Jenoptik.

Her research is dedicated to advancing ultrafast science and technology with advancements in ultrafast solid-state and semiconductor lasers, utilizing semiconductor saturable absorber mirrors (SESAMs) and achieving ultrashort pulse generation in the one to two optical-cycle regime with frequency comb generation and stabilization. She applied these lasers to conduct attosecond experiments testing fundamental processes in quantum mechanics and pioneered the attoclock technique.

Her awards include the Swiss Science Prize Marcel Benoist (2022), OSA Frederic Ives Medal (2020), SPIE Gold Medal (2020), IEEE Edison Medal (2019), OSA Charles H. Townes Award (2015), EPS Senior Prize (2011), and two ERC advanced grants (2012 and 2018). Keller has supervised 94 Ph.D. students, authored 516 journal articles, and holds an h-index of 122 with over 55,000 citations according to Google Scholar. In 2022, she authored a new graduate textbook on "Ultrafast Lasers" published by Springer Verlag.



Roberto Gomez Calvet

Universidad Europea de Valencia, Spain

Roberto Gómez Calvet is a permanent lecturer in the business department of the European University of Valencia. He also lectured for 14 years at the University of Valencia and works regularly with the Polytechnic University of Valencia and the University of La Laguna. In the research field, his current lines of work deal with energy and the environment together with efficiency models using non-parametric techniques. He has written various articles and chapters of books about eco-efficiency, promoting variable renewable energies and fitting them into the electrical grid. His most recent papers concern the energy transition in Spain, published in high-impact journals including Renewable and Sustainable Energy Reviews, Applied Energy, Renewable Energy, European Physical Journal Plus and Energies. He is an honorary senior research fellow at De Montfort University (Leicester, UK).

He trained as an industrial engineer, specialising in energy techniques, at the Polytechnic University of Valencia, holds a degree in Economics and Business from the University of Valencia, an MBA from APD and a doctorate in Economics from the Jaume I University of Castelló. In the professional sphere, it should be highlighted that since the 90s he has held responsible positions in different companies in the Valencia region. He continues to combine his academic and professional careers, seeking points of convergence and cooperation between university, business and society. Also, in recent years he has been active in the media, including press, TV and radio, informing about matters relating to energy, the environment and decarbonisation of the economy.



Yolanda Prezado **Institut Curie, France**

Yolanda Prezado is a research director at the French National Center for Scientific Research (CNRS) and head of the interdisciplinary team New Approaches in Radiotherapy (NARA), based at Institut Curie (France). She has a multidisciplinary background. She received her Ph.D. in Physics from the University of Santiago de Compostela, Spain, in 2003. She is a Medical Physics expert (board certified in Spain and France). She did her Medical Physics residency at Hospital of Salamanca (Spain, 2004-2007), and later worked at Hospital of Pamplona until she was recruited as a beamline scientist at the Biomedical Beamline at the European Synchrotron Radiation Facility. Since 2011 she has been a permanent scientist at the CNRS.

Her main interests are innovative radiotherapy techniques, combined radio-immunotherapies, radiobiology, and small field dosimetry. Her main focus are spatially fractionated radiation therapy and proton therapy. One of their main projects is proton minibeam radiation therapy, funded by the European Union via an ERC consolidator grant. She has been the chair of the scientific committee of the European Federation of Medical Physicists from 2019 to 2021 and is the deputy spokesperson of the International Biophysics Collaboration. She has served on many committees and working groups. Her work in proton therapy has been rewarded with the Mr et Mme Peyre prize of the French Academy of Sciences in 2021.



Olga Smirnova **Max Born Institute, Berlin**

Olga Smirnova graduated from the Physics Department of the Moscow State University in 1996 and received her PhD there in 2000, continuing as assistant professor. In 2003 she received the Lise-Meitner Fellowship of Austrian Science Foundation (FWF) and joined the Vienna University of Technology as a postdoctoral fellow. In 2005 she moved to the National Research Council (NRC) in Ottawa, Canada, where she became a permanent staff scientist in 2006.

In 2009 she received the SAW award of the Leibniz society and moved to the Max Born Institute to establish her own Strong Field Theory research group, which she continues to lead. Since 2016 she also holds full professorship at the Technical University Berlin. In 2010 Olga has received the Karl-Scheel-Preis of Physikalischen Gesellschaft zu Berlin, in 2020 the Ahmed Zewail Award in Ultrafast Science & Technology of the American Chemical Society and in 2022 Mildred Dresselhaus Prize. Olga's current research focuses on imaging and control of ultrafast electron dynamics in atoms, solid state materials, and molecules, especially chiral molecules. Her research has been recently supported by the Horizon Europe ERC advanced grant.



Juan Ignacio Cirac

Max Planck Institute for Quantum Optics, Germany

El profesor Cirac se graduó en Física por la Universidad Complutense de Madrid en 1988 y doctorado en 1991.

Tras ser profesor en las universidades de Castilla-La Mancha e Innsbruck (Austria), es desde 2001 director en el Instituto Max Planck de Óptica Cuántica (Garching, Alemania) y profesor honorario de la Universidad Técnica de Munich.

Cirac es uno de los pioneros del ordenador cuántico. Su investigación se centra en la teoría cuántica de la información y en computación cuántica. Ha recibido diversos premios que incluyen el Premio Nacional de Investigación Blas Cabrera en 2007, el Premio Fundación BBVA Fronteras del Conocimiento 2009, la Medalla Franklin 2010, la Medalla Niels Bohr 2013, Premio Wolf (2013), el Premio de Física Teórica de la Ciudad de Hamburgo en 2015, la Medalla Max Planck de la Sociedad Alemana de Física en 2018, el Premio John Stuart Bell de la Universidad de Toronto y el Micius Quantum Prize de la Fundación Micius (China) en 2019.



Javier Aizpurua

Centro de Física de Materiales, Spain

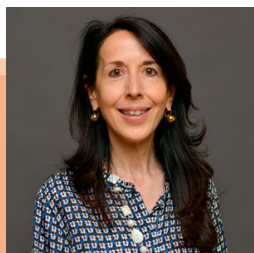
Javier Aizpurua is an Ikerbasque research professor at Donostia International Physics Center (DIPC) in San Sebastián and distinguished researcher at the University of the Basque Country, leading the "Theory of Nanophotonics Group", where he studies interactions between light and matter at the nanoscale. He previously worked at the Center for Materials Physics of CSIC, Chalmers University of Technology in Sweden, and the National Institute of Standards and Technology (NIST) in the US. He has published more than 200 works on the topic of nanoplasmonics, particularly in the area of nanoantenna-enhanced microscopy and spectroscopy, with particular emphasis on quantum surface effects in plasmonics.



Ricardo Díez-Muiño

Centro de Física de Materiales & Donostia International Physics Center

Ricardo Díez Muiño holds a PhD degree in physics by the University of the Basque Country. He further developed his scientific career at the University of Bordeaux (France) and at the LBNL (Berkeley, USA). Díez Muiño later joined, as a CSIC researcher, the Centro de Física de Materiales (CSIC-UPV/EHU) where he served as Deputy Director (2005 – 2011) and Director (2011 – 2015). He is currently Ikerbasque Professor and Director (since 2013) of the Donostia International Physics Center. His main fields of research are chemical physics and condensed matter theory, in particular molecular dynamics at surfaces, the theory of electronic excitations, and the theory of photoemission and photoelectron diffraction. He has published more than 120 scientific articles, as well as two books. Díez Muiño has been the organizer or coorganizer of 5 international conferences. He is Vicepresident of Euskampus Campus of Excellence, Board Member of CIC nanoGUNE, and very active in science communication activities.



Alessandra Buonanno

CERN & Max Planck Institute for Gravitational Physics

Alessandra Buonanno is a director at the Max Planck Institute for Gravitational Physics. She specializes in modeling gravitational waves from binary systems of black holes and neutron stars, aiming to address open questions in cosmology, astrophysics, and gravity. Her research on waveform modeling has been instrumental in the detection and physical interpretation of gravitational waves with LIGO and Virgo detectors. Buonanno pioneered and greatly contributed to the successful synergistic approach of combining numerical-relativity techniques with analytical-relativity methods with the goal of developing the most accurate and efficient waveform models for gravitational-wave observations.

Alessandra Buonanno studied theoretical physics in Pisa, and held faculty positions in Paris and at the University of Maryland, where she became professor in 2010. She is a Principal Investigator of the LIGO Scientific Collaboration and a Research-Unit Head of the Einstein Telescope Collaboration. She is a member of the LISA Consortium Board. For her contributions to gravitational-wave research, she was awarded several prizes, including the 2018 Gottfried Wilhelm Leibniz Prize – the most prestigious research prize in Germany. In 2021 she was co-awarded the Galileo Galilei Medal, the Dirac Medal, and the Balzan Prize.

She received the 2022 Tomalla Prize for her outstanding work on gravitational-wave physics, and the 2023 Oskar Klein Medal. She is an elected member of the German National Academy of Sciences Leopoldina, the US National Academy of Sciences, the Italian National Academy Lincei, and the Berlin-Brandenburg Academy of Sciences and Humanities. Buonanno is a Fellow of the International Society on General Relativity and Gravitation and of the American Physical Society. She holds a research professorship at the University of Maryland, and honorary professorships at the Humboldt University in Berlin, and at the University of Potsdam.



Jorge Mira

Universidad de Santiago de Compostela, Spain

Jorge Mira Pérez is a full professor of electromagnetism at the faculty of physics of the University of Santiago de Compostela (USC). His research has focused on materials science, dynamics of social systems, medical-related areas, and electrical and civil engineering. He has been recognized, among others, with the 2022 Galician Medal of Research. He was head of the department of applied physics at USC, advisor to the Spanish ministry of science for the creation of the International Iberian Nanotechnology Lab (INL), member of the committee of experts of the Galician government on Covid-19 and member of the commission of experts of the government of Spain for the reform of the official time.

He is also active in science communication in mass media (television, radio, newspapers), writing books or leading several activities, such as the Program ConCiencia, developed with the participation of Nobel laureates. He has been recognized, among others, with the 2023 Prize of the Confederation of Scientific Societies of Spain for the dissemination of science.



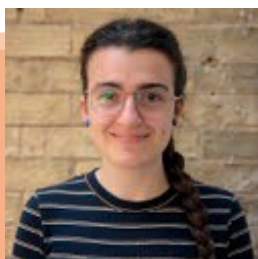
Pedro Miguel Etxenike

Presidente del Donostia International Physics Center (DIPC)

President of the Donostia International Physics Center (DIPC), he is Professor of Condensed Matter Physics at the University of the Basque Country, Honorary President of Jakiunde (Academy of Sciences, Arts and Letters), founding President of the Nanogune Cooperative Research Center (CIC) and of the Materials Physics Center (MPC). He holds a degree in Physics from the University of Navarra, a Ph.D. from the Universities of Cambridge (1976) and Aut3noma de Barcelona (1977), a postdoc at Oak Ridge National and a Nordita fellow in Lund and Copenhagen. He was Minister of Education and Culture and spokesman of the Basque Government (1980-1984).

Member of the Royal Academy of Sciences, the Academy of Sciences and Letters of Milan and the Académie Royale de Belgique. He has been overseas fellow at Churchill College and visiting professor at the Cavendish Laboratory, Cambridge. Fellow of the American Physical Society (APS) and the American Association for the Advancement of Science (FAAAS). He has been a member of the Trilateral Commission (1996-2015).

He is the author of more than four hundred publications in specialized journals and books. He has received several awards, among others Euskadi, Dupont, Príncipe de Viana de la Cultura, Max Planck, Premio Príncipe de Asturias de Investigación Científica y Técnica, Iberdrola, Nacional Blas Cabrera. He has been distinguished with the Grand Cross of Alfonso X the Wise, the Gold Medal of Navarra, of Guipúzcoa, of the Royal Society of Physics, of the University of the Basque Country and of the University of the Basque Country.



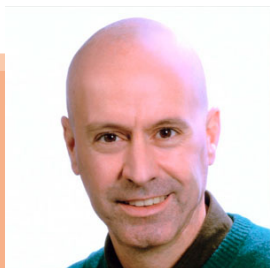
Irene Abril Cabezas

Instituto de Astronomía de la Universidad de Cambridge

Irene is a PhD candidate in Applied Mathematics and Theoretical Physics at the University of Cambridge, specialising in cosmology. Her research uses the lensing signal imprinted on the cosmic microwave background to learn more about structure growth in the Universe. She works as part of the Atacama Cosmology Telescope and Simons Observatory collaborations.

Irene holds a Bachelor's Degree in Physics from Universidad Complutense de Madrid and a Master in Advanced Studies in Astrophysics from the University of Cambridge, graduating top of her class in both degrees. During this time, she also interned at various institutes across Asia and Europe, including the University of Oxford (UK), the Max-Planck-Institute for Astrophysics (Germany) and Academia Sinica Institute for Astronomy and Astrophysics (Taiwan).

In 2022, she was the winner of the V WONNOW Women in Science and Technology Awards. As a strong advocate for increasing the number of women in STEM, Irene participates in numerous outreach events and gives interviews in local media.



Francisco Savall

Teacher of Physics and Chemistry at IES Veles e Vents at Grau, Gandía

Francisco Savall Alemany has a degree in Physics by the University of Valencia (UV) and a PhD by the University of Alicante (UA). He has been awarded in 2023 with the RSEF-Fundación BBVA Award for Physics Teaching and Dissemination in the category of Secondary Education. He currently teaches Physics and Chemistry at IES Veles e Vents at Grau de Gandia. For more than 10 years he has combined his work as a high school teacher with teaching and research as associate professor at the University of Alicante, being member of the Research Group in Didactics of Experimental Sciences.

His main field of research is the development of innovative materials for Physics teaching, many of which have been published in prestigious national and international journals. As a result of this work, he has given teacher training courses aimed at improving Physics teaching in secondary and high school.

Francisco Savall also carries out physics dissemination activities. In this field, he participates assiduously with his students in the Experimenta Science Fair, in which they have been awarded in 2024, he has published several dissemination science articles and is member of the editorial board of the science dissemination magazine DAU AL DEU.



Jorge Méndez

Professor of Applied Physics at Universidad de La Laguna (Tenerife, Canary Islands, Spain)

Professor of Applied Physics at Universidad de La Laguna (Tenerife, Canary Islands, Spain) and researcher in luminescent materials with “rare earth” elements and in the applications of nanotechnology and photonics to renewable energies (solar energy, “green hydrogen”, “artificial photosynthesis”). Principal Investigator of the “MAGEC-REsearch” Project (“Materials for Advanced Energy Generation in the Canary Islands and exploration of rare-earth resources”), financed by the Ministry of Economy and Competitiveness of Spain and by the Research Agency of the of Canary Islands Government.

The project is focused, on the one hand, on exploring the “rare earth” mineral resources in the Canary Islands and, on the other hand, on the development of photonic applications of the latest generation, from the improvement of photocatalysis and generation of solar fuels to the development of luminescent security inks. He has 100 scientific publications in prestigious international journals, three six-year periods of research, as well as three industrial patents on luminescent nanomaterials with technological applications. President of the International Organizing Committee of the SHIFT series of international conferences on light applications in renewable energy and biomedicine, www.shifttenerife.com. Responsible for the weekly scientific dissemination program “Pura Ciencia” that has been broadcast on the air in prime time in the morning within the program “Hoy por Hoy” Tenerife (Cadena SER Radio Club Tenerife) and “Hoy por Hoy El Drago” (SER Las Palmas) since July 2021 and continues today. Scientific disseminator and organizer of scientific culture events, among others, around the figure of Blas Cabrera Felipe, physicist considered “father of Spanish physics.”

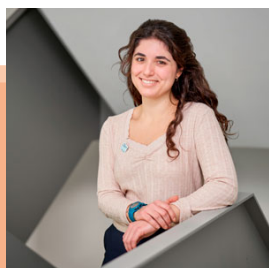


Verónica Sanz
Professor at University of Valencia (Spain)

Veronica Sanz is a full Professor of at the University of Valencia (Spain), and previously at Sussex (UK). Originally from Valencia, she worked at MIT, Harvard, Yale, Boston, York and Durham universities, besides her hometown university and CERN (Geneva).

Her main research line is on Particle Physics, to answer questions such as the genesis of our Universe, and what it is made of. To pursue these research goals, mathematical models need to be developed and contrasted with Nature's behaviour in experiments. This comparison often involves the use of sophisticated numerical techniques, such as AI.

Besides her activities in fundamental physics, Sanz works on broader questions like the understanding of intricate ecological interactions, the polarization of political discourse or the understanding of Art from an AI perspective.



Inmaculada Pérez Pérez
Scientific assistant at the Friedrich-Schiller-Universität Jena

Inmaculada holds a B.Sc. in Physics from Universidad de Sevilla and an M.Sc. in Photonics from the Friedrich-Schiller Universität Jena, Germany, where she specialized in nanophotonics and nonlinear optics. Currently, she works as a scientific assistant at the Friedrich-Schiller-Universität Jena, where she merges the fields of quantum optics and nanoplasmonics to understand the generation of entangled photon pairs, crucial for quantum technologies.

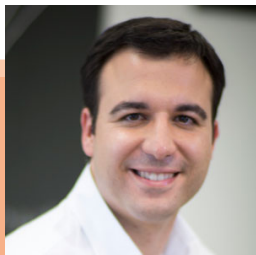
Dedicated to fostering a diverse scientific network, Inmaculada has been an active member of RSEF's Students Group (Grupo de Estudiantes) since its foundation in 2018. She has held various positions within the group's directive board -including secretary, treasurer, and vice president- and is also engaged in other renowned international scientific societies such as Optica and SPIE. This experience has provided her with a broad overview of the evolving role of young physicists in the 21st century, who increasingly navigate multidisciplinary teams and bridge the gap between academia and industry.



Itziar Otegui
Outreach Manager at CIC nanoGUNE

Itziar Otegui, Outreach Manager at CIC nanoGUNE since 2012, has coordinated the design and implementation of the Gender Equality Plan at the research center. She graduated in Humanities and Communication at the University of Deusto, and earned a postgraduate degree in Science Journalism and Science Communication from the UNED.

She is specialized in corporate communication and science communication. In addition to managing the corporate communication and outreach programs of the research center, she has participated in the creation and coordination of several outreach and STEAM education projects, such as 10alamos9 and Nanokomik. She participated in the creation of the Emakumeak Zientzian (Women in Science) initiative in 2017, and has coordinated several of its editions. At nanoGUNE she also coordinates the co-curricular training of research staff, participated in the constitution of the Gender Equality Committee of the center and is responsible for the implementation of the GEP.

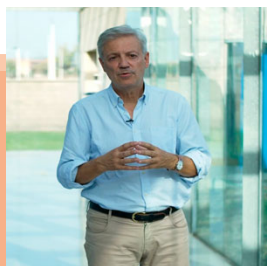


Jorge Bravo

Professor in the Condensed Matter Theory Department and the Condensed Matter Physics Center (IFIMAC) at Universidad Autónoma de Madrid (UAM)

Jorge Bravo-Abad is currently a professor (Profesor Titular) in the Condensed Matter Theory Department and the Condensed Matter Physics Center (IFIMAC) at Universidad Autónoma de Madrid (UAM). He earned his Ph.D. in Physics at UAM in 2006 and conducted postdoctoral research at MIT from 2007 to 2010. Returning to UAM as a Ramón y Cajal Fellow in 2010, he became a faculty member of the Condensed Matter Theory Department in 2016. He served as a Visiting Associate Professor (Fulbright Scholar) in the Physics Department of MIT during the 2018-2019 academic year.

His research group focuses on discovering fundamentally new concepts, theoretical approaches, and physical phenomena at the crossroads of condensed matter physics, materials science, and machine learning. Committed to education, Jorge Bravo-Abad has been instrumental in integrating artificial intelligence into the scientific curriculum at UAM. In 2020, he founded the Spanish Network for AI in Condensed Matter Physics and Materials Science, uniting over 30 academic and industrial research groups to foster the adoption and innovation of AI in condensed matter physics and materials science.



José Luis Sánchez Gómez

Director of the Environment Research Institute of the University of Leon and vice president of the Spanish Meteorological Association (AME)

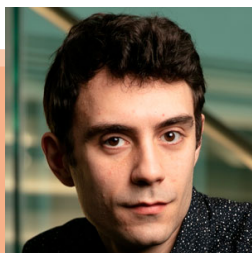
Born in Segovia, he earned his Ph.D. in Physics at University of Valladolid in 1983. Since 2003 he has been Professor of Applied Physics at the University of León. He has been a professor at the University of Valladolid, a visiting professor at the U. Paul Sabatier (Toulouse, France) and at the U. of Barcelona (Spain) and has also taught doctoral degrees at three universities in Brazil. He has been the director of the thesis of 15 Ph. Ds.

He is the main PI of a scientific research group whose main objective is the meteorology of severe weather situations, a leading group in hail precipitation research. Likewise, the group has specialized in aeronautical meteorology in which it has achieved some milestones related to aeronautical safety.

He has published more than 120 scientific articles in international journals and has more than 200 communications at conferences. PI of 22 R&D&i projects earned in competitive calls and in more than 50 research contracts with national and foreign companies and public entities.

He has been Editor-in-Chief of the Journal of Atmospheric Research for 10 years. He has received some awards and decorations, among which I highlight the cross for aeronautical merit awarded by the Ministry of Defense.

He is currently director of the Environment Research Institute of the University of Leon, vice president of the Spanish Meteorological Association (AME) and until December 2023 has been president of the Spanish-Portuguese federation of meteorological societies (Flismet).



Claudio Zeni

Senior Researcher at Microsoft Research Cambridge

Claudio Zeni is currently a Senior Researcher at Microsoft Research Cambridge, contributing to the AI4Science initiative.

He received his Ph.D. in computational physics at King's College London in 2020, and subsequently worked as a post-doctoral researcher at the International School for Advanced Studies (SISSA) before joining Microsoft Research in 2022.

His research is focused on leveraging artificial intelligence to broaden our toolkit for addressing environmental issues, specifically within the field of materials science. His work involves the development of methods for discovering new materials, understanding their atomic-level behavior, and predicting their properties. His expertise includes machine learning force fields, generative models for crystals, and molecular dynamics simulations.

As an active participant in the scientific community, Claudio has organized several conferences on machine learning for materials science and has had the opportunity to present his research in many conferences around the world.



Jonathan Home

Professor of Experimental Quantum Information at ETH Zurich

Jonathan Home has been a Professor at ETH Zurich since 2010, when he established the Trapped-Ion Quantum Information group. He moved to ETH Zurich following post-doctoral research at NIST Boulder, working on a Lindemann Fellowship in the group of Dave Wineland. His undergraduate and graduate studies were performed in Oxford, the latter under the supervision of Prof. Andrew Steane. Jonathan Home's research focusses on quantum state engineering and control with atomic systems, primarily trapped ions. The group has produced pioneering work across a range of areas, including first demonstrations of continuous feedback stabilization of entangled states based on in-sequence measurements, dissipative protocols for state stabilization, and the first demonstration of full quantum error correction in an ion trap system, using motional states of a single ion. This work has been accompanied by a focus on advanced technology for scaling ion trap systems, including new methods for constructing ion traps, pioneering implementations of quantum gates using integrated photonics and the first loading and quantum manipulation of ions in a new architecture for trapped-ion control based on microfabricated Penning traps. The TIQI group have recently also managed to put barium atoms on display to the public, in a new permanent exhibit at the hands-on Technorama science museum in Winterthur.

Jonathan's research work has been recognized by a number of prizes, including the 2019 Landauer-Bennett award of the APS and the ETH Zürich Latsis prize. In 2023 he was named as an APS Fellow. Jonathan has also been recognised for his contributions in teaching and outreach, including the Golden Owl of ETH Zürich and being named as a TED Fellow.

Symposia / Simposio

XXXIII Iberian Meeting for the Teaching and Dissemination of Physics (DEDF) / XXXIII Encuentro Ibérico para la Enseñanza y Divulgación de la Física (DEDF)

Organiser

José María Pastor, Pablo Nacenta Torres, María Fernanda Miguélez Pose, Guilhermina Nogueira, Luis Afonso

Invited speakers

Deolinda Campos (Presidenta de La Divisao de Educaçao) Fernando Nogueira (Universidad de Coimbra)
Manuel Alonso Sánchez (División de Enseñanza y Divulgación de la Física) Jorge Mira Pérez, (Universidad de Santiago de Compostela)

Symposium abstract

The Iberian Meeting of Teaching and Dissemination of Physics is the Symposium organized by the Division of Teaching and Dissemination of Physics (DEDF). It has been developed since 1991 coinciding with the RSEF Physics Biennial, and has its replica in Portugal in parallel with the Physics Biennial of the Portuguese Physics Society (SPF) in even years. It is intended as a meeting point for teachers of all educational levels who are interested in sharing proposals and experiences through oral communications and/or posters on teaching and dissemination topics. As is traditional, at the XXXIII Iberian Meeting current topics and relevance for the teaching of Physics of interest to Secondary Education and University teachers will be discussed.

This edition's program will analyze in depth the current situation of double degrees in Physics, degrees that are already offered by numerous Spanish universities. On the other hand, Organic Law 3/2020 of Modification of the Organic Law of Education (LOMLOE) establishes in its curricular development the specific competencies for the subject of Physics, and in this regulatory framework the need for Education students will be addressed. Secondary school, they must be competent in basic experimental work for learning Physics. This analysis will be completed with the study of the problems inherent to the implementation of the Baccalaureate Assessment for University Access (EBAU) in Physics, proof that in this 2023-2024 school year will focus on the new 2nd year Physics curriculum. Baccalaureate, after its implementation in centers for the first time. The equivalent proof in Portugal will be presented by a representative of the SPF.

El Encuentro Ibérico de Enseñanza y Divulgación de la Física es el Simposio que organiza la División de Enseñanza y Divulgación de la Física (DEDF). Se desarrolla desde el año 1991 coincidiendo con la Bienal de Física de la RSEF, y tiene su réplica en Portugal en paralelo con la Bienal de Física de la Sociedad Portuguesa de Física (SPF) en los años pares. Está pensado como un punto de encuentro para los profesores de todos los niveles educativos que estén interesados en compartir propuestas y experiencias a través de comunicaciones orales y/o poster en temas de docencia y divulgación. Como ya es tradicional, en el XXXIII Encuentro Ibérico se tratarán temas de actualidad y relevancia para la enseñanza de la Física del interés del profesorado de Educación Secundaria y Universidad.

En el programa de esta edición se analizará en profundidad la actual situación de los dobles grados de Física, titulaciones que ofertan ya numerosas universidades españolas. Por otra parte, la Ley Orgánica 3/2020 de Modificación de la Ley Orgánica de Educación (LOMLOE) establece en su desarrollo curricular las competencias específicas para la materia de Física, y en este marco normativo se abordará la necesidad de que los estudiantes de Educación Secundaria, han de ser competentes en el trabajo experimental básico para el aprendizaje de la Física. Este análisis se completará con el estudio de los problemas inherentes a la implantación de la Evaluación de Bachillerato para el acceso a la Universidad (EBAU) en Física, prueba que en este curso escolar 2023-2024 versará sobre el nuevo currículo de Física de 2º de Bachillerato, tras su implementación en los centros por primera vez. La prueba equivalente en Portugal se presentará por un representante de la SPF.

List of abstracts at the symposium

La SPF Y La Educación Básica y Secundaria en Portugal

1st author

Maria Deolinda Gonçalves Da Costa Campos Agrupamento De Escolas Alberto Sampaio

Abstract

A Sociedade Portuguesa de Física (SPF), constituída em 1974, tem contribuído para a melhoria da qualidade do ensino da Física, nos ensinos básico e secundário (EB/S). Nesta comunicação, destacam-se os contributos relacionados com:

a divulgação científica de interesse para alunos e professores na Gazeta de Física;

o incentivo e o desenvolvimento do gosto pela Física nos alunos dos EB/S, organizando anualmente as Olimpíadas Nacionais de Física e promovendo a participação de equipas portuguesas na International Physics Olympiad e na Olimpíada Ibero-americana de Física;

a formação de alunos do ES, atualmente, através do projeto MEDEA, promovendo a medição e o conhecimento de campos elétricos e magnéticos de muito baixa frequência, a construção de experiências sobre esses campos e a pesquisa sobre eventuais efeitos desses campos na saúde humana;

a formação de professores dos EB/S, organizando, desde 1978, conferências de Física (desde 2000, integram encontros ibéricos para o ensino da Física), e, desde 2010, ações de formação;

a avaliação externa das aprendizagens dos alunos, tendo representação no Conselho Consultivo do Gabinete de Avaliação Educacional/Conselho Científico do Instituto de Avaliação Educativa, auditando, desde 2007, a componente de Física de provas de exame/aferição, com emissão de pareceres prévios sobre essas provas relativos ao rigor científico, à adequação aos documentos curriculares de referência, ..., elaborando propostas de resolução detalhadas das provas de exame, desde 2008, e pareceres sobre essas provas, a posteriori, desde 2012;

a avaliação e certificação de manuais escolares, de modo a garantir a qualidade científica e pedagógica dos manuais a adotar [...], tendo equipas científico-pedagógicas da SPF avaliado e certificado no total sete manuais;

as aprendizagens essenciais das disciplinas da área disciplinar de Física e Química, elaboradas pela Direção-Geral de Educação, desde 2016/2017, em parceria com equipas de professores indicados pela SPF e pela SPQ.

PANEL: Situación de los dobles grados de Física en las universidades españolas

Authors

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Carmen Carrión Pérez Universidad de Granada

Idoia García de Guturbay Galligo Universidad del País Vasco

A low cost device to demonstrate the magnetic force between parallel wires

1st author

Manuel Iván González Martín Universidad de Burgos

Abstract

This work describes a nearly zero-cost device, manufactured using DIY techniques, intended to reveal the weak magnetic force between two parallel wires. The device is easily portable to the classroom. A unique auxiliary instrument is required: a DC power source capable of supplying a few amperes. By changing the electrical connections it is possible to quickly switch between the modes of parallel and antiparallel currents. The device has already been successfully used in the classroom, with first-year undergraduate students and final-year secondary school students.

Behavior of low frequency magnetic fields induced by electrical cables

1st author

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Abstract

This communication describes an experimental setup to studying the decay behavior of magnetic fields induced by anti-parallel electrical conductors as a function of the distance between them. The aim is to demonstrate in the laboratory the behavior of electrical power transmission lines, leading to an understanding of the more abrupt decay of the field in a bifilar cable when compared to a single one.

The experimental setup consists of an electrical extension with two fixed cables separated with a certain distance. This extension will be used to power various types of household appliances with variable intrinsic powers to cause the flow of various currents in both cables.

A protocol is presented that allows the use of experimental setup to identify the law of magnetic field decay, demonstrating the near-limit situation of nearby cables. The experiment allows us to understand what extent the distance between the conductor cables defines the decay function. The results are presented in three different situations. For the mathematical decay model the MSExcel Solver is used which allows determining the function that best fits the experimental data.

It is possible to conclude that since the two cables are practically in contact with each other, the decay law is proportional to $1/r^2$ and the near field quickly extinguishes. If the cables are far apart, their decay in the proximity of one of the conductors varies only with $1/r$, which implies the existence of a much higher near field. The experience also makes it possible to understand the concept of near field and far field by interpreting the distances at which measurements are carried out in terms of the main distance of the experiment, that is, the distance between the conductors, putting the geometry of the problem into perspective.

Transistores de alta potencia: cómo transmitir su importancia al público general

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Abstract

Uno de los principales objetivos para una sociedad más sostenible es el uso racional y eficiente de energías renovables y la red eléctrica. En el camino desde la generación hasta su consumo, la energía eléctrica es

transformada varias veces (de continua a alterna, cambios de voltaje, cambios de frecuencia...). En cada etapa, la conversión eficiente de electricidad requiere el uso de transistores de muy alta potencia (1200 V, 100 A). Es importante por tanto transmitir al público general la necesidad de investigar nuevos materiales y diseños que permitan gestionar altas potencias a un coste asequible. Sin embargo, los conceptos técnicos y el lenguaje científico requeridos son difíciles de entender. En nuestra propuesta destacamos el papel de los nuevos materiales comparando el tamaño de los transistores tradicionales de silicio con transistores de nitruro de galio, mucho más pequeños debido a sus propiedades superiores de conmutación y conducción eléctrica y térmica. Como aplicación del uso de transistores en la vida cotidiana se muestra el funcionamiento de una cocina de inducción. En cuanto a su aplicación industrial, se ha realizado un montaje de alta potencia para el calentamiento por inducción de piezas ferromagnéticas. En él pueden visualizarse claramente los transistores empleados en el circuito resonante. Las tres demostraciones permiten comprender la utilidad del fenómeno físico de inducción y conectan el uso de transistores con la experiencia cotidiana.

Acknowledgments: This project has received funding from the ECSEL Joint Undertaking (JU) under grant agreement No 101007229. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, France, Belgium, Austria, Sweden, Spain, Italy. Also financed by the European Union-NextGenerationEU, PCI2021-121970/ AEI / 10.13039/501100011033.

Incorporación de la perspectiva de género en la enseñanza y divulgación de la física

1st author

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Abstract

La inclusión de la perspectiva de género en la educación universitaria es fundamental en todas las áreas donde los temas, resultados y aplicaciones de los contenidos impactan de manera directa en individuos, como miembros de la sociedad, o de forma indirecta a través de la forma en que las instituciones y organizaciones regulan las interacciones sociales. De la misma manera cualquier forma de comunicación debe tener en cuenta la igualdad y la inclusión, y así es importante abordar la incorporación del enfoque de género en la divulgación de la física. La física es una de las áreas STEM cuyos porcentajes de alumnas en bachillerato y en el grado universitario se encuentra alrededor del 25%, y desafortunadamente estos porcentajes están disminuyendo o se encuentran estancados desde hace más de 15 años. Para aumentar las cifras, es importante desterrar la visión androcéntrica de la cultura de la física, a menudo cargada de connotaciones masculinas a nivel simbólico (ejemplos, metáforas que pueden ser sexistas y refuerzan los estereotipos de género), y esa construcción limitada y limitante de la física ha dificultado que muchas mujeres encuentren un lugar en la disciplina. A menudo se habla de la ceguera de género en la docencia y la divulgación, ya que las mujeres han estado presentes en la construcción científica del conocimiento desde los orígenes mismos de la Ciencia, aunque la Historia –escrita secularmente por varones y sobre varones– las haya mantenido invisibilizadas y al margen de los libros de texto oficiales. En esta contribución animaremos a revisar los contenidos docentes para identificar los sesgos androcéntricos en las asignaturas, así como facilitar recomendaciones, informes, estrategias equitativas en aula, y recursos para el profesorado. Estos contenidos también servirán para abordar una comunicación científica en física más igualitaria.

IA y aprendizaje basado en problemas: Potenciando el éxito en estudiantes de posgrado

1st author

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Abstract

En los últimos años, la intersección entre la inteligencia artificial (IA) y la educación ha surgido como un área crucial de exploración, redefiniendo paradigmas pedagógicos tradicionales y remodelando el panorama del aprendizaje estudiantil y la participación en la investigación. La utilización de herramientas de IA tiene un potencial inmenso para mejorar la experiencia de aprendizaje, especialmente en estudios de posgrado, donde el desarrollo del pensamiento crítico y las habilidades de investigación son primordiales. A través de metodologías de aprendizaje basado en problemas, los educadores pueden aprovechar el poder de la IA para facilitar experiencias de aprendizaje estructuradas que capacitan a los estudiantes para navegar por dominios de investigación complejos con confianza y competencia.

Además, los enfoques habilitados por IA ofrecen nuevas vías para promover la participación activa de los estudiantes en entornos de aula. Al integrar herramientas de IA como ChatGPT en marcos instructivos, los educadores pueden crear entornos de aprendizaje dinámicos que fomenten la investigación colaborativa, la evaluación entre pares y el discurso intelectual. A través de la integración efectiva de tecnologías de IA, es posible cultivar una cultura de investigación e innovación, capacitando a los estudiantes para convertirse en agentes activos en su propio viaje de aprendizaje.

En este trabajo, presentamos diferentes enfoques utilizando herramientas de IA que pueden ser utilizadas como herramientas de visualización de redes para ayudar a estudiantes de doctorado y de grado en un escenario del mundo real para la revisión de literatura (como Citation Gecko o Connected Papers); para aprovechar la IA y el aprendizaje basado en problemas; para fomentar el análisis crítico y la comunicación científica en estudiantes de posgrado (usando plataformas como Elicit o Jenni) y para mejorar la participación estudiantil en el aula mediante la evaluación efectiva de la calidad de trabajos de investigación (usando ChatGPT). Este trabajo tiene como objetivo ser una revisión de diferentes herramientas impulsadas por IA y su integración dentro de marcos de aprendizaje basado en problemas para mejorar significativamente los resultados estudiantiles en ciencias y más allá.

“Melhoria da Qualidade das Aprendizagens no ensino da Física”

1st author

Guilhermina Do Carmo De Almeida Nogueira Sociedade Portuguesa de Física

Abstract

Ensinar Física não se resume a transmitir conhecimentos restritos nem mesmo a trabalhar conteúdos de Física!

De acordo com as aprendizagens essenciais | articulação com o perfil do aluno: “Deve-se ensinar Física para que os alunos compreendam fenómenos naturais e dispositivos tecnológicos (como forma de interpretar o mundo), para que apreendam a essência do conhecimento científico e as suas consequências para a sociedade, a tecnologia e o ambiente, para preparar escolhas profissionais e para o exercício de uma cidadania plena.”

O AEPA tem como Missão: Promover aprendizagens de qualidade, no respeito pela inclusão e diversidade de escolhas; Contribuir para a formação de cidadãos responsáveis, autónomos, solidários e interventivos, capazes de responder aos desafios colocados pela sociedade do conhecimento.

No 12º ano os alunos desenvolvem projetos que se consubstanciam em conceber e desenvolver experiências concretas, de qualidade, relacionadas com as suas áreas de interesse pessoal e/ou vocacional.

Recorriendo a metodología do traballo de projeto – recollen, analizan, seleccionan información, resollen problemas, toman decisións adecuadas, justificando esas decisións e comunicando-as, por escrito e oralmente, utilizando suportes diversificados, nomeadamente as novas tecnoloxías da información/comunicación, articulando, numa dimensión interdisciplinar e transdisciplinar, os saberes teóricos e prácticos.

O espazo físico do Clube de Ciencia Viva aePA e a axuda do InovLabs “startup educacional de aconsellamento a escolas e profesores na implementación da educación STEM” posibilitan a extensión das tarefas en tempo e en aprofundamento das aprendizagens.

Global e regularmente, os alumnos:

- Consolidan, aprofundan e amplían o coñecemento en contexto experimental;
- Desenvolven hábitos e competencias inherentes ao traballo científico: observación, pesquisa de información (seleccionar, analizar, interpretar e avaliar criticamente información relativa a situacións concretas), experimentación, abstracción, xeneralización, previsión, espírito crítico, resolución de problemas e comunicación de ideas e resultados, utilizando formas variadas;
- Desenvolven competencias de recoñecer, interpretar e producir representacións variadas da información científica e do resultado das aprendizagens. Ensinar Física é, con base en exemplos concretos, articular o coñecemento e o saber facer asociado a capacidade de pensar de forma crítica e creativa.

Galileo en un autobús urbano

1st uthor

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Abstract

Una de las posibles dificultades de aprendizaje en Física es el esfuerzo prematuro por desarrollar la formulación matemática de los modelos, descuidando su conexión con la realidad empírica. Pueden producirse aprendizajes con resultados satisfactorios en determinadas pruebas de evaluación, vinculados a la resolución de problemas, compatibles con profundos errores conceptuales (1-3). En la enseñanza de la Mecánica de Newton suele concedérsele una relevancia reducida a la 1ª Ley, algunas veces mostrada como un caso particular de la 2ª.

Se presenta un video con observaciones en contextos inerciales y no inerciales al estilo de las de Galileo en sus Diálogos (4). El navío se ha sustituido por un autobús urbano reconectando con la realidad empírica que conduce a la 1ª Ley, y con la experiencia previa con que inician el aprendizaje formal los estudiantes. Se persigue su carácter significativo, que permita afianzarlo visual, matemática y verbalmente (5). La Unidad de Cultura Científica de la Universidad de Burgos ha editado el video, que ha sido utilizado en varios institutos de enseñanza secundaria en el curso 2023-2024; el material es válido para 1º de grado en ingenierías. La efectividad del aprendizaje se ha determinado con una versión modificada del Force Concept Inventory (1)

(1) D. Hestenes, M. Wells, and G. Swackhamer, Force Concept Inventory, Phys. Teach. 30, 141 (1992).

(2) D. Huffman and P. Heller, What does the Force Concept Inventory actually measure?, Phys. Teach. 33, 138 (1995).

- (3) D. Hestenes and I. Halloun, Interpreting the Force Concept Inventory: A response to March 1995 critique by Huffman and Heller, Phys. Teach. 33, 502 (1995).
- (4). G. Galilei. Diálogos sobre los dos máximos sistemas del mundo. Ed. MAXTOR. ISBN: 9788497617390. 2010
- (5) J. Handhika¹, C. Cari and A. Suparmi. Students\' representation about Newton law: consequences of "zero intuition" 2017 J. Phys.: Conf. Ser. 795 012057

Active methodologies in 1st year Physics: improving student's performance, motivation and intuition

1st author

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Abstract

We present an overview of the impact of introducing active methodologies in the teaching of the 1st year Physics courses in the Physics degree, Electronic Engineering degree and double degree in Physics and Electronic Engineering in the University of the Basque Country (UPV/EHU) since the Bologna process (2010/2011 in UPV/EHU). Because of the large number of students enrolled in these courses, we started using formative evaluations via Moodle quizzes. They were initially mandatory and later were left at the students' judgment to use them as self-evaluation tools. We found that those who passed the quizzes, increased the probability of passing and obtained on average better marks. Later we introduced simple experiments related to daily life at the beginning of each topic. When anonymously questioning the students about the outcome of the experiment, we found that they systematically showed wrong preconceptions, and their physical intuition failed. This has been quite surprising not only for the lecturers, who sometimes wrongly assume that students have more intuition and knowledge than they do, but also for the students, who become aware of their weaknesses. Only then do they start wondering about the physics behind the experiment. This, hopefully, acts as a catalyst for increasing their motivation towards the topic they are studying. After every topic, we reevaluate their knowledge on the related concepts and find that a higher percentage of the students answers correctly. We also report on a PBL experience to motivate and engage them by showing that the Physics they learn can explain many simple daily-life phenomena. Finally, we show the results of a flipped classroom. 90% of the students find these activities motivating and useful. Unfortunately, lately we have found little engagement from the students to do prior work at home, which makes it difficult to carry out these activities successfully.

El acceso a la Universidad en Portugal

1st author

Fernando Nogueira Universidad de Coimbra

PANEL: El nuevo currículo de Física en las aulas y en la EBAU. ¿Transformación o continuismo?

Authors

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Bachillerato de Investigación: una colaboración entre Secundaria y Universidad. Un ejemplo sobre el estudio de propiedades físicas de espesantes

1st author

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Abstract

El “Bachillerato de Investigación” es una propuesta del IES Dr. Peset Aleixandre que forma parte del Plan de Actuación para la Mejora (PAM) llamada “Fomento del Talento”. Se ofrece al alumnado de 1º de Bachillerato la posibilidad de realizar una investigación colaborando con profesorado de la Universidad o investigadores.

El alumnado elige tema o campo de conocimiento de forma libre y una comisión del IES creada a tal efecto, asigna un tutor entre el profesorado de las materias afines. El tutor acompaña al alumno en todo el trabajo (resuelve dudas, revisa entregas...) y la propia comisión forma al alumnado (una sesión semanal) en aspectos como: estructura de un trabajo académico, búsqueda de hipótesis, o citas bibliográficas. Todo el proceso contará con el asesoramiento de colaboradores externos, expertos en el tema, que acabarán de definir y guiar el trabajo.

En el caso presentado la idea partió de la Fira Experimenta 2021 donde el equipo de Jorge Ortega participó con un trabajo sobre tensión superficial en líquidos (premio en “Demostraciones Físicas en la ESO”). Con la idea de continuar estudiando propiedades físicas de líquidos, se contactó con M^a Jesús Hernández y se decidió finalmente realizar un análisis de la viscosidad sensorial e instrumental de diferentes espesantes alimenticios usados para pacientes con disfagia. El desarrollo teórico y la parte experimental se inició en los laboratorios del IES y se completó en el laboratorio de Reología Aplicada de la Universitat de València.

El trabajo se defiende en público delante de un tribunal y el instituto publica los trabajos, hace difusión y los considera en la calificación final de la materia más afín (en este caso, “Física y Química”). El trabajo de Jorge se presentó los Premios Sapiència de investigación 2023 y obtuvo el primer premio en la categoría: “Matemáticas, Física y Química”.

Evaluación por competencias en Física de Bachillerato Internacional

1st author

Patricio Gomez Lesarri IES Ramiro de Maeztu

Abstract

El Diploma de Bachillerato Internacional es una modalidad de Bachillerato reconocida internacionalmente, impartida desde 1968 y regulada por la Organización del Bachillerato Internacional (IBO en inglés). De

acuerdo con sus postulados educativos, su objetivo es proporcionar una formación integral a sus alumnos que les permita desarrollar su propia personalidad y fomentar su capacidad de aprender a aprender. Para obtener el Diploma, los alumnos deben cursar 6 asignaturas a lo largo de 2 cursos y realizar una monografía centrada en una de ellas, bajo la supervisión de un profesor. La enseñanza de Física se desarrolla en dos posibles niveles, el medio y el superior, en los que se exige un número mínimo de clases experimentales. Aunque los contenidos incluidos en el currículo son similares a los establecidos por el sistema educativo español, la evaluación que realiza el Bachillerato Internacional presenta diferencias sustanciales con la que se aplica en la actual EVAU/EBAU. Algunas de estas características distintivas son las siguientes:

- Realización obligatoria de una investigación experimental de física, evaluada internamente en el propio centro educativo, pero moderada externamente para garantizar la homogeneidad de la calificación
- Inclusión de elementos de calificación variados, tales como ejercicios numéricos, cuestiones teóricas, preguntas conceptuales, tanto de contestación corta como extensa
- Uso del análisis de datos experimentales, gráficas, tablas de datos, etc.
- Contextualización de las preguntas en situaciones extraídas de la vida cotidiana, aplicaciones tecnológicas, prácticas deportivas, etc.
- Evaluación de la capacidad de relacionar la física con otras áreas de conocimiento Por estas razones, el sistema de evaluación de Física en el Diploma del Bachillerato Internacional podría ser una referencia para desarrollar la evaluación por competencias que establece la actual legislación educativa española en la LOMLOE. Bibliografía
- IBO (2024). Comprender la evaluación en el PD

Los ODS a través de la física: feria experimenta y colección de demostraciones

1st author

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Abstract

Los desafíos a los que se enfrenta la humanidad y que motivan la agenda 2030 y los Objetivos de Desarrollo Sostenible (ODS) pasan por una auténtica comprensión de la ciencia y de su papel en nuestras vidas. Una educación científica de calidad no sólo es necesaria para formar adecuadamente a futuros físicos y físicas, quienes desarrollarán los ODS a través de iniciativas y proyectos. Es necesaria también para la ciudadanía, y en particular para contrarrestar el negacionismo y la transmisión de bulos que se oponen a los ODS como objetivos legítimos. Es importante enfatizar el método científico, las evidencias y su relación con las teorías que predicen multitud de fenómenos y de desarrollos tecnológicos, y no solo los resultados finales. Este espíritu y planteamiento se encuentra implícito en dos iniciativas de enseñanza y divulgación que cuentan con una larga trayectoria y que se proponen como formas de desarrollar y vehicular los ODS en un contexto formativo universitario, en la enseñanza secundaria y la divulgación a todo tipo de público. La colección de demostraciones experimentales, dispositivos sencillos que se pueden usar en el aula para observar (en vivo y en directo), permite discutir y entender fenómenos, estableciendo una enseñanza con más interacción y diálogo con el alumnado. La feria-concurso Experimenta, tiene como objetivo es fomentar la curiosidad y la observación por lo que nos rodea y la comprensión de la ciencia y la tecnología a través de proyectos STEM experimentales de física y tecnología que el propio alumnado desarrolla y explica al público visitante, realizando una labor de divulgación científica. Ambas iniciativas, con un énfasis en la participación de mujeres, trabajan temas relacionados con el clima, la energía, el ambiente o la salud, de los que se presentan ejemplos, incidiendo en los aspectos metodológicos que los vertebran.

La física en las aulas de principios del siglo XX: Lecciones para el profesorado del siglo XXI

1st author

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Abstract

La investigación en didáctica de la física ha subrayado la importancia de la historia de la física para la enseñanza-aprendizaje de esta ciencia. Sin embargo, la historia de la enseñanza de la física ha recibido una menor atención en el seno de la investigación didáctica. Asimismo, el profesorado de física de enseñanza secundaria suele desconocer la historia del colectivo profesional en el que se integra, más allá de experiencias personales o algunos autores destacados. Por el contrario, la historia de la enseñanza de la física se ha erigido en las últimas décadas como un área fértil de investigación en el marco de los estudios históricos y sociales sobre ciencia. La presente comunicación pretende contribuir a acercar la investigación sobre historia de la enseñanza de la física a la investigación educativa y la práctica docente poniendo el foco en la enseñanza de la física en las primeras décadas del siglo XX. Se trata de un periodo histórico de especial interés debido a la profunda renovación que experimentó la enseñanza de la física en el plano internacional. A través del análisis de la obra de algunos destacados profesores renovadores de la época en España, como el profesor Modesto Bargalló Ardévol (1894-1981), y de algunas publicaciones de entonces, como el boletín Faraday (reconocida como una publicación pionera en España sobre historia y enseñanza de la física), se ofrecerá una análisis de cuestiones sobre didáctica de la física de gran relevancia en el contexto educativo actual, como la relación entre física y química, las conexiones entre física y sociedad, la incorporación de prácticas experimentales a la docencia o el uso educativo de la historia de la física. Además, se presentarán varias experiencias de aula basadas en la recreación de experiencias docentes históricas, como la reconstrucción de un gabinete de física de 1924.

La formación STEM en los grados de Magisterio de Educación Primaria

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Abstract

Actualmente está en marcha una reforma de los Grados de Magisterio en Educación Primaria. Uno de los motivos es adecuarlos mejor a la nueva Ley de Educación (LOMLOE), la cual incluye por vez primera y de manera explícita la competencia STEM. Para poder abordar decisiones a este respecto, este trabajo pretende analizar la formación en las disciplinas STEM en dichos grados. Para ello se analizan las diferentes materias relacionadas con estas disciplinas, su carga en créditos, su carácter más didáctico o más disciplinar y se compara esta tipología entre universidades públicas y privadas. Se han revisado los planes de estudios de las 37 universidades públicas y 22 privadas que ofertaron el Grado de Magisterio en Educación Primaria en el curso 2020-2021, lo que supone un total de 342 guías docentes. Se han detectado diferencias significativas en la temporalización y enfoques de las disciplinas científicas y matemáticas, así como entre tipos de universidades. En cuanto a la tecnología, los contenidos se corresponden con las Tecnologías de la Información y la Comunicación (TIC), y no con la Tecnología entendida desde STEM. Por su parte, la Ingeniería y el propio enfoque global STEM se han mostrado ausentes, a pesar de su ubicuidad en los foros educativos. Se concluye por tanto la necesidad de renovar los planes de estudio con un enfoque más adecuado a la LOMLOE actual, así como incluir aspectos de Tecnología e Ingeniería desde una perspectiva

STEM. Todo ello tendría un efecto en el desarrollo de las etapas educativas posteriores y en la construcción de identidades y vocaciones científico-tecnológicas más inclusivas.

¡Física por favor!

1st author

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Abstract

Presentamos una sección que aparece regularmente en la Revista de divulgación científica DAUALDEU, escrita en valenciano y editada por la asociación cultural Meridià Zero de la Marina Alta (Alicante):

<https://dualdeu.associaciomeridiazero.com/>.

Nuestra sección, dirigida al público en general, cubre desde 2019 diversos campos de la física y la astrofísica, siempre con una visión histórica y social. Algunos títulos significativos son: ¿Se puede viajar a mayor velocidad que la luz? (2020), Hipatia, una loable excepción en la historia antigua de la ciencia (2021), Brahe y Kepler: un encuentro cósmico (2022), De la alquimia a la física nuclear (2023), El descubrimiento del espín y su importancia actual (2024).

El hechizo de las velas: experiencias para diseñar una situación de aprendizaje

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Abstract

Para la adquisición y el desarrollo de las competencias clave, la LOMLOE señala que deben buscarse metodologías que reconozcan al alumnado como agente de su propio aprendizaje.

Mediante la planificación de un conjunto de actividades secuenciadas alrededor del funcionamiento de una vela, se ha creado una *situación de aprendizaje* en la que el alumnado debe dar respuesta a diferentes cuestiones de tipo científico. Por ejemplo, ¿cómo llega un material sólido hasta la llama? ¿A qué son debidas la forma alargada y las diferentes coloraciones de la llama? También deberán enfrentarse a interrogantes asociados a la acción de una vela sobre diferentes dispositivos como una tira bimetalica y conceptos como la conductividad térmica de metales. Señalar que la observación, la descripción y la interpretación sirven de puente de unión de toda la propuesta.

Con el conjunto de actividades se abordan las 6 competencias específicas de la materia de Física y Química en secundaria, y saberes básicos relacionados con las metodologías científicas, la energía, la materia o con el cambio.

La serie de experimentos buscará también responder a la pregunta: ¿Es una herramienta eficaz para alumbrarnos y dar calor? ¿Cómo hacían nuestros antepasados para ver por la noche? y ¿cómo se iluminan los más de 675 millones de personas que no tienen acceso a la electricidad? De esta manera, el *hechizo de las velas* abre un camino para que el alumnado pueda dibujar utopías para construir presentes y futuros deseables, dando un *enfoque eco social* a la propuesta.

«Un video, Galileo»: creación y análisis de un canal de experimentos de física

1st author

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Abstract

Con frecuencia, docentes y futuros docentes señalan factores limitantes para llevar a cabo actividades experimentales en las aulas. Entre ellos, se señala la ausencia percibida de instalaciones, materiales y referentes –a modo de guía– para desarrollar estas actividades; dificultades que se agudizan cuando se propone, además, implementar enfoques basados en la indagación y la modelización. Con la intención de contribuir a subsanar esta situación, en esta comunicación se presenta un canal de experiencias de Física titulado «Un video, Galileo». Este espacio contiene más de 40 videos cortos (2–8 minutos) para ilustrar experimentos secuenciados sobre fuerzas, equilibrio de estructuras, energía, calor y temperatura, máquinas simples, ondas y electromagnetismo. Estas experiencias, que recurren a materiales cotidianos, persiguen finalidades didácticas diversas, tales como: favorecer la expresión de ideas e hipótesis; diseñar estrategias para probarlas; implicar a los participantes en una construcción guiada de modelos; reproducir experimentos históricos; construir explicaciones para fenómenos contextualizados y aplicaciones tecnológicas; y adoptar enfoques de ciencia recreativa. En la actualidad, las experiencias están integradas en los programas de diversas asignaturas del Grado en Magisterio de Educación Primaria y del Máster en Formación del Profesorado de Educación Secundaria de la Universidad de Alcalá, y también han sido difundidas en cursos de formación para docentes en ejercicio. Contamos con resultados que avalan su contribución a la comprensión conceptual de los fenómenos implicados, así como su impacto en la generación de emociones positivas hacia los contenidos abordados. Así pues, en la comunicación se ilustrará una selección de experimentos del canal y se discutirán algunas de las contribuciones antes reseñadas.

Los cursos de formación impartidos por la DEDF

1st author

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Divulgación Para Trasladar los Resultados Científicos a la Gestión Pública

1st author

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La cámara de niebla más allá de la física de partículas. Diseño, construcción y uso de instrumento de detección por parte de estudiantes de bachillerato para trabajar desde la intra e inter disciplinariedad.

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Abstract

El diseño, construcción y uso de instrumentos científicos por el alumnado, permite desarrollar destrezas científicas como la resolución de problemas, la toma de decisiones o el diseño experimental. La enseñanza de la física de partículas en secundaria y bachillerato puede ser abordada como un contexto útil más allá del aprendizaje de los conceptos de la física moderna. Una forma de hacerlo es a través de un instrumento de detección de partículas como la cámara de niebla. Los fundamentos físicos de este dispositivo abarcan distintas ramas de conocimiento, como la termodinámica, las propiedades físico-químicas de los materiales o la óptica. A su vez, si se plantea no solo el uso, sino el diseño y construcción del instrumento por parte del alumnado, se requieren destrezas científicas como las mencionadas, además de conceptos interdisciplinares como la tecnología o la ingeniería. En este contexto se llevó a cabo una investigación con 64 estudiantes de 1º de bachillerato, durante 6 sesiones en un instituto de Zaragoza. Los estudiantes trabajaron en grupos y con la bibliografía aportada, debían diseñar, conseguir los materiales y construir sus propias cámaras de niebla. Se realizó una sesión de observación de partículas en la que probaron sus dispositivos y debían recoger los datos de observación mediante la grabación de vídeos. Los estudiantes diseñaron y construyeron sus propias cámaras de niebla, recogiendo en un diario de aula las dificultades encontradas, su resolución y la justificación de las decisiones. En la observación, se comprobó que no todos los dispositivos de los estudiantes funcionaban correctamente. En algunos casos, pudieron identificar los problemas y resolverlos, pero no en todos. Finalmente, todo el alumnado tuvo la oportunidad de observar partículas y grabarlas en vídeo para su análisis. En conclusión, la construcción y uso de las cámaras de niebla por el alumnado permitió trabajar conceptos sobre la física de partículas y también el desarrollo de habilidades científicas esenciales. Estas actividades ofrecen una vía efectiva para trabajar conceptos intra e interdisciplinares tanto en la física como en otras áreas de conocimiento.

Break out como herramienta en la enseñanza de la Física

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Abstract

La innovación docente es un aspecto fundamental a trabajar para captar el interés de nuestro estudiantado y fomentar el aprendizaje significativo de los conceptos más importantes de la Física.

En las últimas décadas se han propuesto y se están llevando a cabo diferentes metodologías activas en el aula, las cuales están dando lugar a una mayor implicación, participación, interés y mejores resultados en el proceso de enseñanza-aprendizaje dentro de nuestro sistema educativo.

En nuestro caso, hemos propuesto, a través de la metodología de la gamificación, un “Break Out Educativo” para estudiantes de 2º y 3º de ESO, para trabajar de forma novedosa, motivadora, activa y colaborativa las propiedades de la materia; en concreto, se indaga y se practica el concepto de densidad. Además, con esta actividad se trabajan otras competencias transversales como la expresión oral y escrita y el uso de las TIC.

El “Break Out Educativo” se inicia con la visualización de un video de un atraco a una joyería a modo de introducción. A continuación, se expone el caso explicando que se ha acusado a un mafioso de ser el autor del robo y para demostrar su inocencia, han secuestrado a los estudiantes ya que pertenecen a la policía científica. Para ello, el capo les ha brindado un par de instrumentos de laboratorio para demostrar la autenticidad de las joyas de plata presuntamente robadas y tienen 40 minutos para llegar a una respuesta.

En primer lugar, el alumnado tiene que averiguar qué propiedad de la materia puede ser utilizada para resolver el caso y, posteriormente, tienen que utilizar los instrumentos de laboratorio para determinar la masa y volumen de las joyas con el fin de calcular la densidad, y compararla con la de la plata real, demostrando así la culpabilidad o inocencia del mafioso.

Problemas de Campo Eléctrico para contribuir a desarrollar la competencia científica

1st author

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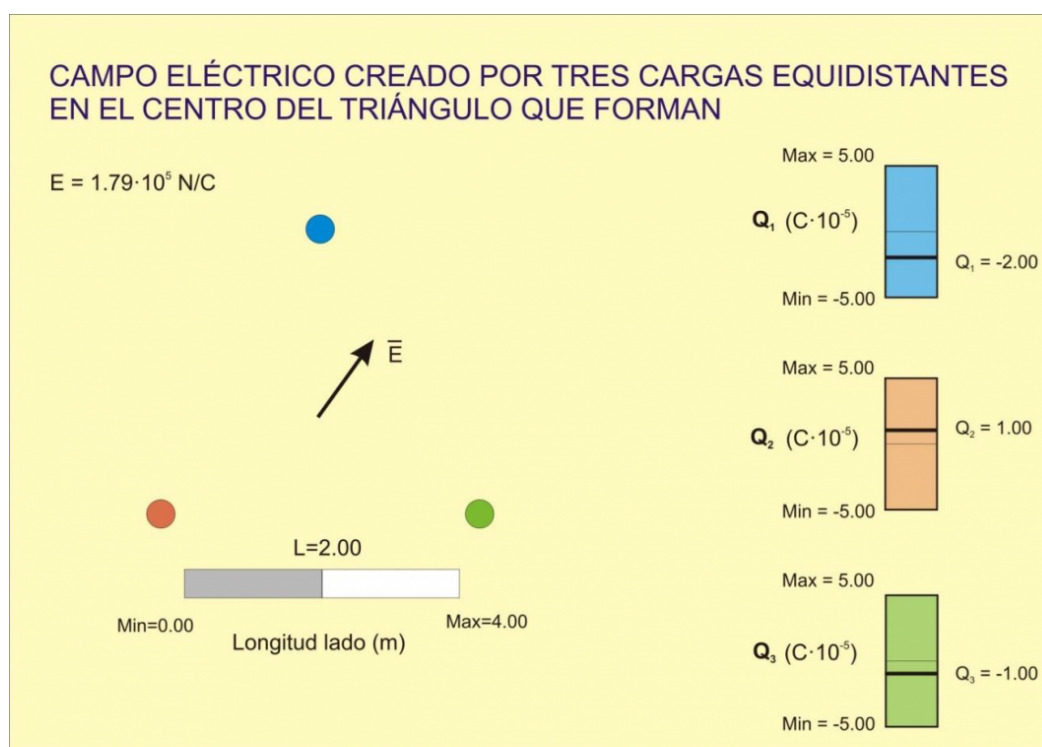
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Abstract



Presentamos una colección amplia de problemas resueltos sobre Campo Eléctrico, que son apropiados para el nivel de Bachillerato y primeros cursos de Universidad. Se ha realizado una resolución cuidadosa de los mismos, contextualizada en un modelo de enseñanza de las ciencias por investigación orientada [1]. Dicho modelo implica, por lo que se refiere a la resolución de problemas, promover que el alumnado: tome conciencia del interés e importancia de la situación problemática abordada, realice un planteamiento cualitativo inicial, operativice la situación problemática precisando cuál es la magnitud buscada, emita razonadamente hipótesis acerca de las variables intervinientes, avance algunos casos límite de fácil interpretación, intente elaborar diversas estrategias de resolución, se embarque en la resolución propiamente dicha siguiendo dichas estrategias, analice detalladamente el resultado (literal) obtenido, plantee nuevas perspectivas, posibles ampliaciones, etc. Todo ello es esencial para poder contribuir eficazmente desde la resolución de los problemas al desarrollo de la Competencia Científica [2],

Los problemas están a disposición del profesorado en abierto [3, 4] y, muchos de ellos, se han enriquecido con animaciones informáticas interactivas de elaboración propia, que pueden usarse libremente en cualquier ordenador y con las cuales los estudiantes pueden contrastar de manera visual sus hipótesis (modificando el valor de cada parámetro y viendo cómo se altera o no el resultado), pueden analizar (cualitativa y cuantitativamente) el resultado, etc.

En la ponencia oral desarrollaremos, paso a paso, uno de los problemas y manipularemos su animación, para mostrar en un ejemplo concreto la plausibilidad y potencialidad del modelo.

[1] Gil, D. (1983). Tres paradigmas básicos en la enseñanza de las ciencias. *Enseñanza de las Ciencias*, 1 (1), 26-33.

[2] Carrascosa, J., Martínez, S. y Alonso, M. (2020) Competencia Científica y Resolución de Problemas de Física. *Revista científica*, vol.38, nº2 (<https://revistas.udistrital.edu.co/index.php/revcie/article/view/16211>)

[3] <http://rsefalicante.umh.es/fisica.htm>

[4] <http://didacticafisicaquimica.es/>

Super Teacher Mario - Didactical situations within a Super Mario video game to reinforce Physics concepts among bachillerato students

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Abstract

Super Mario is the most widely known video game character. Nintendo's plumber has starred so many games, that most of us have enjoyed them at some point. Most of them are platform games, whose most attractive aspect is the role that physics plays in them, having led some researchers to investigate them [1].

Considering that video games are popular among teenagers, their use in education has increased over time [2]. We have designed a project, set in the video game "Super Mario Galaxy", in order to exemplify and reinforce Physics concepts among bachillerato students.

This project uses gamification as a resource, similar to what we did in a previous work by means of an escape room [3]. In this activity, didactical situations are identified during the exploration of the game's world, making emphasis on the physical phenomena involved, carrying out experimental activities and solving questions, so that students consolidate Physics concepts learned in the classroom.

This project aims to help students to avoid conceptual errors in Physics that may difficult the learning of this subject at university, awakening interest in learning playfully and encouraging cooperative work. This project has been carried out with the bachillerato students at IES Severo Ochoa (Elche) and with the collaboration of some teachers from other areas.

[1] C. Sullivan, J. Sallabank, A. Higgins, A. Foden, "It's a me Density!", *Journal of Physics Special Topics*, Oct 8, 1-2, 2014.

[2] F. J. Martínez, F. del Cerro, G. Morales, "El uso de Minecraft como herramienta de aprendizaje en la Educación Secundaria Obligatoria", *Claves para una educación diversa*, Murcia: Consejería de Educación, Cultura y Universidades, 2014.

[3] A. Avila, J. Martínez-Asencio, P. de Vera, "Quantum Break: un escape room para reforzar conceptos de Física y Química en Bachillerato", *Revista Española de Física*, 37-2, 30-33, 2023.

POSTER: Estudio de viabilidad para la transición de MatLab al lenguaje de programación Python en Física y Matemáticas

Presenter

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Co-presenters

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Miguel Villaplana Pérez Institut de Física Corpuscular (IFIC), University of Valencia and CSIC

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Abstract

El objetivo de esta contribución es mostrar como se ha realizado un estudio de viabilidad para llevar a cabo la transición desde MatLab al lenguaje de programación Python en la asignatura de Métodos Numéricos y Estadísticos impartida en segundo del grado en Física y tercero del doble grado en Física y Química de la Universitat de València.

Los objetivos específicos están consistiendo en escribir primero en Jupyter Notebook y python algunos ejemplos actuales utilizados en dichas asignaturas actualmente basados en Matlab, para que puedan ser ejecutados directamente por los estudiantes.

El uso de Python en el desarrollo de la asignatura permitirá en un futuro ampliar fácilmente su contenido e incluir nociones prácticas para la aplicación de los distintos métodos de aprendizaje profundo en la resolución de diferentes tipos problemas relacionados con la asignatura.

POSTER: GeoGebra como herramienta para realizar prácticas virtuales de física

Presenter

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Abstract

Este trabajo es un homenaje a nuestro compañero Jenaro Vera Guarinos que fue el precursor de estas prácticas en los tiempos de la pandemia y que nos dejó en 2021.

Uno de los problemas más acuciantes que tuvo el profesorado de física con la llegada de la pandemia y el confinamiento fueron las prácticas de laboratorio. Dicho problema continuó el curso siguiente cuando únicamente una parte del estudiantado podía asistir a las clases y el resto seguía las clases desde casa de manera virtual. Estas situaciones sobrevenidas nos hicieron buscar alternativas para que el estudiantado pudiera adquirir el máximo de destrezas y competencias de las que estaban previstas en las respectivas guías docentes de las asignaturas.

Una de estas alternativas ha sido la simulación de los experimentos con el programa Geogebra que es un programa libre, cuya condición es que, una vez realizados los programas, estos son accesibles para el resto de los usuarios. Por otra parte, hemos detectado que a parte de la ventaja evidente de poder hacer medidas utilizando las simulaciones de manera no presencial, existen prácticas cuya realización en el laboratorio tiene dificultades evidentes que el programa puede ayudar a evitar. Uno de los ejemplos más claros puede ser la interacción entre imanes, dicha práctica se realiza en las asignaturas de fundamentos físicos de las ingenierías, dichas asignaturas están ubicadas en los primeros cursos de los grados. En este caso concreto existe la dificultad que, debido a la repulsión de los polos iguales, para el estudiantado es dificultoso medir con exactitud la distancia a la que están los imanes, por lo que los resultados experimentales obtenidos en muchos casos no se aproximan a los predichos por la teoría. Para finalizar el estudio, se han pasado encuestas para tener la opinión del estudiantado.

POSTER: Familiarizándose con el dominio de frecuencias: Filtrado paso-bajo en lentes Fibonacci

Presenter

Sergi Gallego Rico University of Alacant

Co-presenters

Juan Carlos Bravo University of Alacant
Jaume Colomina-Martínez University of Alacant
Joan Josep Sirvent-verdú University of Alacant
Guillem Nájjar University of Alacant
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Víctor Navarro-Fuster University of Alacant
Antonio Hernández University of Alacant
Augusto Beléndez University of Alacant

Abstract

La sucesión de Fibonacci sigue siendo muy popular entre el estudiantado, aunque ya hace más de veinte años que el libro “El código Da Vinci” con más de setenta y nueve millones de ventas la encumbrara hacia el “Mainstream”. De hecho, sólo poner algunas de las imágenes icónicas relacionadas con esta sucesión en el proyector, y es reconocida casi al instante por la mayoría del estudiantado. Por lo tanto, su efecto motivador es innegable, todo un tesoro para un docente.

Últimamente se ha demostrado que las lentes difractivas de fase basadas en la sucesión de Fibonacci tienen propiedades bifocales [1]. Es decir, presentan dos planos focales cuyos focos están en el eje óptico. Esta propiedad hace que sean especialmente prometedoras para diversas aplicaciones, incluidos los avances potenciales en oftalmología, especialmente en el tratamiento de la presbicia.

Pues dichas lentes se pueden registrar de una manera bastante sencilla en fotopolímeros, y en el montaje experimental propuesto enviamos la distribución de intensidades de la lente Fibonacci a un modulador espacial del tipo LCOs y la proyectamos en el fotopolímero utilizando un sistema 4F.

En el plano de la transformada de Fourier, es decir, en el plano focal de las dos lentes que componen el sistema se coloca un diafragma que hace de filtro paso-bajo, cambiando el diámetro de la apertura se puede controlar el filtrado, de esta manera al quitar las frecuencias altas, se ve en tiempo real como la focal corta es la que se ve enseguida afectada por el filtrado paso-bajo.

[1] Ferrando Martín, V.; Calatayud Calatayud, A.; Andrés, P.; Torroba, R.; Furlan, WD.; Monsoriu Serra, JA. (2014). Imaging Properties of Kinoform Fibonacci Lenses. IEEE Photonics Journal. 6(1):65001061-65001066. <https://doi.org/10.1109/JPHOT.2014.2304560>

POSTER: Inteligencia artificial en la enseñanza de Física en estudios de ingeniería: percepciones y aplicación

Presenter

J.j. Suñol University of Girona

Abstract

En lo que respecta a la innovación docente, una de las temáticas que está generando más frentes de análisis y de discusión es el de la aplicación de la inteligencia artificial, IA, en procesos de aprendizaje y evaluación. En este trabajo se analiza la aplicación de la inteligencia artificial en la enseñanza de Física en estudios de Ingeniería. Por una parte, se han realizado encuestas entre estudiantes de primer curso sobre la percepción y el grado de conocimiento de la IA. En general, son más partidarios de su aplicación en procesos de aprendizaje y de evaluación que en procesos de evaluación dirigidos por el profesorado. Un porcentaje significativo de estudiantes está preocupado por su futura incidencia en el mercado laboral. La aplicación práctica de la IA se ha realizado en actividades de trabajo en equipo y en la generación de material docente. Se ha comprobado la tendencia generalizada de la IA a: a) proporcionar información no suficientemente contrastada, b) dar bibliografía incorrecta o c) no estar suficientemente preparada para actividades de carácter científico o tecnológico (incluso en versiones de pago de la IA).

En la generación de material docente se ha constatado que fácilmente proporciona material incorrecto y que, si quien interactúa no es un experto, el material docente generado puede ser contraproducente. Se muestran algunos ejemplos. Evidentemente, el sistema está en evolución y se acabarán generando sistemas tutores inteligentes. Además, como profesorado tenemos que ser conscientes que los alumnos actuales son usuarios de la IA, pero en pocos años los estudiantes de primer curso ya serán nativos en IA.

POSTER: Movimiento de conjuntos de “filtros de café”

Presenter

Maria Deolinda Gonçalves Da Costa Campos Agrupamento de Escolas Alberto Sampaio

Abstract

Da lista das aprendizagens essenciais (AE) de Física e Química A de 11.º ano constam as AE “Interpretar, e caracterizar, movimentos retilíneos (uniformes, [...] e variados) [...], tendo em conta a resultante das forças e as condições iniciais” e “Resolver problemas de movimentos retilíneos ([...] queda com efeito de

resistência do ar não desprezável) [...], aplicando abordagens analíticas e gráficas, mobilizando as Leis de Newton, explicando as estratégias de resolução e os raciocínios demonstrativos que fundamentam uma conclusão.”.

Para estudar um movimento em que a força de resistência do ar não é desprezável, é realizada a atividade laboratorial, em regime de demonstração para a turma, que consiste em deixar cair um “filtro de café” de uma posição que dista cerca de 2 m de um sensor de movimento. Terminada a aquisição automática do gráfico da posição-tempo, repete-se o procedimento para diversos conjuntos de “filtros de café”.

Procede-se então à análise do gráfico posição-tempo correspondente ao movimento de um “filtro de café” e compara-se, por exemplo, com o do movimento do conjunto de quatro “filtros de café”.

Como a força de resistência do ar pode ser considerada diretamente proporcional ao quadrado da velocidade do “filtro de café” (o número Reynolds é elevado) e sendo a impulsão do ar desprezável, pode concluir-se que o quadrado da velocidade terminal (em movimento é retilíneo uniforme) do conjunto de “filtros de café” é diretamente proporcional à sua massa.

Assim, considerando também que os alunos devem ser familiarizados, de modo faseado, com o tratamento de dados experimentais, usando a Estatística da calculadora gráfica traça-se o gráfico do quadrado da velocidade terminal do conjunto de “filtros de café” em função da massa, obtendo-se a respetiva equação da linha de ajuste.

POSTER: Verificação experimental da relação entre a resistência elétrica de um fio de cobre e a temperatura

Presenter

Maria Deolinda Gonçalves Da Costa Campos Agrupamento de Escolas Alberto Sampaio

Abstract

Da lista das aprendizagens essenciais (AE) do subdomínio “Energia e fenómenos elétricos” de Física e Química A de 10.º ano consta a AE “interpretar o significado das grandezas: corrente elétrica, diferença de potencial elétrico e resistência elétrica”, bem como a AE “montar circuitos elétricos, associando componentes elétricos em série e em paralelo [...]”.

Para estudar a dependência com a temperatura da resistência de um condutor filiforme — dependência essa que permitiu o desenvolvimento dos termómetros de resistência — e como se preconiza a promoção de estratégias que envolvam a criatividade dos alunos, por exemplo, para conceber situações onde determinado conhecimento possa ser aplicado, sugere-se a realização de uma experiência, que consiste em medir a resistência da enrolamento de fio de cobre em função da temperatura, colocando-o inicialmente num gobelé com água fria e aquecendo gradualmente a água. Uma vez que é necessário efetuar um número significativo de medições, que se estendem ao longo de um período de tempo considerável, recomenda-se o uso de sensores.

Durante a execução da experiência, recorrendo a uma calculadora gráfica ligada a um sensor de temperatura e a um sensor de tensão elétrica através de uma interface e a um multímetro em função amperímetro (a corrente elétrica mantém-se praticamente constante durante a recolha de dados), foram obtidos os gráficos, que permitem concluir acerca da dependência da resistência de um fio metálico com a temperatura, sem a necessidade de recorrer a quaisquer expressões.

Contudo, essa dependência pode ser também verificada efetuando o tratamento de dados experimentais que conduzem ao gráfico da resistência elétrica em função da temperatura e a respetiva equação da linha de ajuste, permitindo que os alunos se familiarizem, de modo faseado, com o tratamento de dados.

POSTER: Erasmus Summer School on Physics at the UV: Promoting scientific talent from high school

Presenter

María Jesús Hernández Lucas Facultat de Física. Universitat de València

Co-presenters

Alejandro García-Ten Facultat de Física. Universitat de València

Enric Valor Facultat de Física. Universitat de València

José María Martí Facultat de Física. Universitat de València

Abstract

From 2019, the Faculty of Physics of Valencia University has been organizing a five-day school addressed to students of Physics and related degrees from all over Spain and open to the participation of European universities. The School also aims to attract high-school students interested in Physics and Science. The covid-2019 pandemic prevented the normal development of the School in 2020 and 2021, but in recent years it has regained its vitality, helped by the Erasmus programme grants through the BIP (Blended Intensive Programme).

The organising committee of the School consists of physics teachers, researchers and students (including members of RSEF-UV student chapter). The School allows participants (mainly undergraduate students and a selection of high-school students) to enjoy a first experience in a scientific congress-like environment, and offers them the opportunity to present their own contributions as oral presentations and posters.

The School offers lectures, round tables, and some leisure and educational activities in an inclusive and participatory environment. Each year, the scientific programme focuses on a different field of Physics. In the last edition ("From the Earth to the edge of the Universe", 4-8 September 2023), School's programme included lectures both on Astronomy and Astrophysics, and Earth Physics and Thermodynamics as well as contributions on other topics (Gender and Physics, Stress management in university students, Physics and Music, Physics didactics, scientific dissemination,...) by young researchers, PhD students and guest lecturers. As an Erasmus school, it aims at opening up to the European sphere. Last year School was attended by teachers and students from universities of Jyväskylä (Finland), Johannes Gutenberg (Mainz, Germany), and Palermo (Italy), all of them FORTHM Alliance universities.

About a hundred participants are expected to attend the next edition of the School "Unveiling the secrets of matter and light", to be held from 9 to 13 September 2024.

POSTER: Vayas donde vayas, vallas. La tensión superficial: un símil para un enfoque social de la Física

Presenter

Pablo Nacenta Torres División de Enseñanza y Divulgación de la Física

Co-presenter

Jorge Nacenta Mendivil CEA, LETI, Universidad de Grenoble

Abstract

La LOMLOE incluye como seña de identidad la promoción de sociedades más justas, democráticas y sostenibles. En junio de 2023, 110 millones de personas habían sido forzadas a abandonar sus hogares. De ellas, 36,4 millones huyeron a través de las fronteras, escapando de la violencia, la persecución o la guerra. Utilizando los conceptos de tensión superficial, fuerzas de adhesión y cohesión como herramientas, se

propone una serie de experimentos como hilo argumental que busca llamar a la reflexión sobre impacto de estas situaciones de tensión social y sus consecuencias.

La huida. Una gota de jabón (bomba) cayendo sobre una superficie de agua con pimienta (personas) provoca la dispersión de esta.

El naufragio. Se añaden progresivamente polvos de talco sobre un vaso de agua que contiene jabón líquido, hasta provocar su hundimiento (como un bote en el mar con sobrecarga) tras alcanzar el límite de tensión superficial.

El miedo. Al llenar con agua una botella de plástico con 6 pequeños agujeros, se generan varios chorros que se unen al pasar el dedo gracias a las fuerzas de cohesión. ¿Viajar juntos o separados?

Las fronteras, las vallas. Al introducir un cubo hueco hecho con alambre en una disolución jabonosa aparecen diferentes fronteras, pero con la misma composición a ambos lados. ¿Para qué queremos entonces dichas fronteras?

Campo de refugiados. Con una malla en la apertura de un matraz erlenmeyer boca abajo es posible bloquear una gran cantidad de agua en su interior. Las alambradas no dejan salir, y generan mucha tensión.

La indiferencia y el rechazo social. Es posible añadir varias cerillas sobre el extremo de un cartón en equilibrio en el borde de un vaso con agua, gracias a las fuerzas de adhesión entre el cartón y el agua. ¿Qué hace romper el equilibrio social?

POSTER: A second-rank tensor equation for rolling processes

Presenter

Julio Güémez Universidad de Cantabria

Co-presenter

José Ángel Mier Universidad de Cantabria

Abstract

Rolling processes involving linear translation with rotation, including thermal effects, are analyzed by a second-rank tensor equation $\frac{d}{dt} J^{\mu\nu} = M^{\mu\nu} + M^{\mu\phi} \omega^{\nu}$ formalism. This covariant momenta equation is a relativistic generalisation of the angular-impulse--angular-momentum variation equation $\frac{d}{dt} \mathbf{J} = \mathbf{M}$, and the four-vector fundamental equation $\frac{d}{dt} E^{\mu} = \Delta W^{\mu} + \Delta Q^{\mu}$. Poincaré-Euler's law (angular momentum), Newton's second law (linear momentum) and the first law of thermodynamics (energy) are included within the postulated cause-effect formalism. A sophomore physics course characteristic process is described by this formalism: a ring rolling, on a horizontal surface, due to the action of a pair of forces together with the force provided by the ground, fulfilling the rolling condition (mechanical energy conservation).

POSTER: Aprendiendo óptica usando elementos de fase geométrica

Presenter

Pas García Martínez Universitat de València

Co-presenter

Ignacio Moreno Universidad Miguel Hernández de Elche

Abstract

Los elementos de fase geométrica (GPE) se están convirtiendo en atractivos componentes ópticos debido a varios factores: su diseño delgado y plano, su eficiencia, su capacidad para manipular la fase, corregir aberraciones y controlar la polarización. A diferencia de los elementos refractivos convencionales, que requieren un grosor considerable y superficies curvas para manipular la luz, los EPG no están basados en la refracción de la luz. Además, en comparación con los elementos difractivos de fase tradicionales que usan variaciones locales del relieve o el índice de refracción, los EPG emplean el fenómeno conocido como fase de Pancharatnam-Berry. Este desplazamiento de fase puede generarse considerando una distribución geométrica del eje óptico de un retardador, que puede producirse bien con materiales propiamente anisótropos, en concreto cristales líquidos, o bien con metamateriales en los que se índice una birrefringencia artificial. En la actualidad existen redes de difracción y lentes difractivas comerciales basadas en estos materiales, dependiendo de si las distribuciones espaciales de los ejes directores siguen un patrón radial (lente) o cartesiano (redes). En esta comunicación, abordaremos diferentes conceptos que forman parte de la materia “óptica”, como la reversibilidad de los rayos, la formación de imágenes, la difracción e interferencias, o la polarización de la luz, utilizando sencillos montajes ópticos haciendo uso de estos elementos GPE. Presentaremos resultados experimentales que avalarán la propuesta.

POSTER: Typst, un nuevo lenguaje de marcado ligero para la docencia de la Física

Presenter

Alberto Corbi Universidad Internacional de La Rioja (UNIR)

Abstract

El conocido sistema de edición de documentos basado en macros LaTeX se ha convertido en el estándar a la hora de transmitir información escrita en el ámbito de nuestra disciplina. La mayoría de revistas científicas exigen su uso a la hora de recibir artículos. LaTeX posee una capacidad sin parangón para crear bellos documentos con estructura y tipografías consistentes.

En la docencia de la Física, LaTeX se utiliza a menudo para producir notas de clase, presentaciones e informes de laboratorio. Su flexibilidad y la gran cantidad de recursos disponibles han hecho de él un estándar en comunicación científica que los alumnos, incluso de enseñanzas medias, deben ir conociendo. En contrapartida, tiene una curva de aprendizaje empinada, una sintaxis farragosa y un oxidado ecosistema de herramientas con casi medio siglo a sus espaldas.

En los últimos años han emergido potenciales sustitutos a este sistema de edición. Todos ellos están basados en los así llamados lenguajes de marcado ligero: sistemas de escritura con una sintaxis sencilla para agregar formato y estructura al texto plano. Estos lenguajes son comunes en la creación de páginas web y documentos técnicos.

De todos ellos, el que firmemente se está postulando como sucesor de LaTeX es Typst: un nuevo lenguaje de descripción de textos y su compilador asociado. En contraste con LaTeX, el conjunto de herramientas está basado en estándares informáticos modernos y el propio lenguaje posee una sintaxis más limpia y legible y orientada a generar documentos computables (que pueden cambiar según el input proporcionado en tiempo de generación). Typst también utiliza estructuras de programación conocidas en lugar de macros difíciles de entender.

En el grado en Física de la Universidad Internacional de la Rioja se está implantando con éxito este sistema de composición tanto en ejercicios de clase como en trabajos de fin de grado.

POSTER: Densímetros centenarios: del olvido al protagonismo

Presenter

María Matilde Ariza Montes IES "Pedro Espinosa"

Abstract

DENSÍMETROS CENTENARIOS: DEL OLVIDO AL PROTAGONISMO

INTRODUCCIÓN

Durante el siglo XIX, la industria de instrumentos científicos ganó muchos adeptos debido a todos los avances científicos que estaban ocurriendo desde la revolución científica. La industrialización hizo que no sólo las empresas se hicieran eco de la fabricación de nuevos instrumentos sino que la ciencia también tomó partido, aportando a la sociedad nuevos diseños y funcionalidad.

Como consecuencia, el IES "Pedro Espinosa" de Antequera (Málaga), fundado en 1928, atesora una colección de instrumentos científico-históricos correspondientes a todos los campos de la Física.

Este estudio se centra en la puesta en valor de los instrumentos relacionados con la medida de la densidad, tales como balanzas de Mohr-Westphal, picnómetros y densímetros que alberga este instituto histórico, responsables de las prácticas docentes en las aulas del siglo XIX y principios del siglo XX, hoy en desuso por las nuevas ideas pedagógicas. Sin embargo, su importancia fue crucial y novedosa en el siglo XIX para justificar la calidad de líquidos, tales como la leche, y descartar el comercio de bebidas adulteradas que se inició con la era industrial.

PROCEDIMIENTO Y RESULTADOS

En este trabajo, se ha procedido a la identificación y cuantificación de los densímetros centenarios que alberga el patrimonio del IES "Pedro Espinosa", para su puesta en valor, teniendo en cuenta parámetros como la escala, su rango, la temperatura de referencia, las dimensiones o el calibrado, entre otros. Al mismo tiempo, se ha indagado en las características de las balanzas de Mohr-Westphal y los picnómetros.

Una aplicación ha sido el estudio de las densidades de las bebidas lácteas y vegetales, tan imprescindibles en la vida diaria, por sus componentes nutricionales.

Todos los densímetros examinados están calibrados para una temperatura de 15°C y la gran mayoría utilizan el mercurio como contrapeso, correspondiendo éstos a los denominados como aerómetros Baumé y densímetros según peso específico.

POSTER: Enseñanza, aprendizaje y evaluación en Física y Matemáticas con las nuevas tecnologías de la información y la comunicación

Presenter

Miguel Villaplana Pérez Facultat de Física de la Universitat de València

Co-presenters

Santiago Gonzalez De La Hoz Facultat de Física de la Universitat de València

Javier Vijande Asenjo Facultat e Física de la Universitat de València

Facundo Ballester Pallarés Facultat e Física de la Universitat de València

María Moreno LLácer Facultat e Física de la Universitat de València

Juan de Dios Zornoza Gómez Facultat e Física de la Universitat de València

Martín GONZÁLEZ ALONSO Facultat e Física de la Universitat de València

Abstract

El objetivo principal de esta contribución consiste en explicar como se ha implementado una base de datos de preguntas accesible vía web que ha sido utilizada tanto por estudiantes como por docentes. La base de datos está integrada en el entorno virtual de la Universitat de València basado en Moodle y aprovecha la funcionalidad introducida por la herramienta JazzQuiz. Este nuevo sistema se ha diseñado primero para la asignatura de Métodos Numéricos y Estadísticos del Grado en Física y se explicará en esta presentación y en el futuro se exportará a otras asignaturas en futuros proyectos.

X International Workshop on Mathematical Foundations of Quantum Mechanics and its applications (DFTP) / X Taller Internacional sobre Fundamentos Matemáticos de la Mecánica Cuántica y sus aplicaciones (DFTP)

Organiser

Alberto Ibort (ICMAT & UCIIM), Juan Manuel Pérez Pardo (UCIIM), Fabio Di Cosmo (UCIIM), Florio Ciaglia (UCIIM), Laura Bravo González (UCIIM), Arnau Mas (ICMAT), María Jiménez-Vázquez (UCIIM)

Symposium abstract

The “International Workshop on Mathematical Foundations of Quantum Mechanics and its applications” is an international meeting devoted to the study of the mathematical foundations of Quantum Mechanics and their applications, many of them instrumental in the emergent problems related to Quantum Information Technologies. The workshop has been running for more than ten years and past editions have taken place in various locations in Spain and Italy. The objective of this workshop is to present a few relevant problems in the foundations of Quantum Mechanics to a small number of young researchers, Post and Pre doctoral, and to work in a collaborative environment. These problems have been chosen because of their challenging and transversal nature both physical and mathematical.

The subjects that have been highlighted for the present edition of the Workshop are:

- Information Geometry: classical and quantum.
- Foundations of Quantum Mechanics: Schwinger’s picture of Quantum Mechanics.
- Quantum Thermodynamics.
- Foundations of Classical and Quantum Field Theories: categories and groupoids.

The workshop will last for one week and the scientific committee asks some of the participants to prepare an extended exposition accessible to young researchers on the selected subjects.

It is characteristic of this meeting to leave ample time for discussions, favouring the exchange of ideas and stimulating the collaboration among the participants.

El “Taller Internacional sobre Fundamentos Matemáticos de la Mecánica Cuántica y sus aplicaciones” es un encuentro internacional dedicado al estudio de los fundamentos matemáticos de la Mecánica Cuántica y sus aplicaciones, muchas de ellas instrumentales en los problemas emergentes relacionados con las Tecnologías de la Información Cuántica. El taller lleva más de diez años funcionando y en ediciones anteriores se han celebrado en diversas localidades de España e Italia. El objetivo de este taller es presentar algunos problemas relevantes en los fundamentos de la Mecánica Cuántica a un pequeño número de jóvenes investigadores, post y predoctorales, y trabajar en un entorno colaborativo. Estos problemas han sido elegidos por su carácter desafiante y transversal tanto físico como matemático.

Los temas que se han destacado para la presente edición del Taller son:

- Geometría de la Información: clásica y cuántica.
- Fundamentos de la Mecánica Cuántica: visión de Schwinger sobre la Mecánica Cuántica.
- Termodinámica Cuántica.
- Fundamentos de las Teorías de Campos Clásica y Cuántica: categorías y grupoides.

El taller tendrá una duración de una semana y el comité científico pide a algunos de los participantes que preparen una exposición ampliada accesible a los jóvenes investigadores sobre los temas seleccionados.

Es característico de este encuentro dejar amplio tiempo para las discusiones, favoreciendo el intercambio de ideas y estimulando la colaboración entre los participantes.

List of abstracts at the symposium

Mathematical Aspects of Topological Insulators

1st author

Manuel Asorey Universidad de Zaragoza

Co-author

Martinez Yisely Universidad de Zaragoza

Abstract

One interesting characteristic of topological insulators is that their bulk are insulating while their edge are metallic. This striking property is made possible by the appearance of conducting edge states. The quantized conducting properties of these materials are usually characterized by topological indices that either depend either on the bulk observables of the material or on a number of edge states with special characteristics. The amazing coincidence of the two ways of computing the quanta of conductivity is attributed to a mysterious bulk-edge correspondence. The appealing image of such a correspondence has been in some cases related to the AdS/CFT duality arising in string theory which provides the basis for holographic principles. However, the bulk-edge correspondence has never been rigorously proven. In these note we show that the existence of the bulk-edge duality is highly dependent on the physical properties of the material and its boundary conditions. For a large class of boundary conditions the correspondence is a consequence of the continuity of the energy spectrum connecting the bulk and edge states in a smooth manner. However, for APS boundary conditions of the associated Dirac theory such a continuity is broken and the duality bulk-edge does not hold.

Casimir energy on the lattice

1st Author

Fernando Ezquerro Sastre Univ. de Zaragoza

Abstract

When a quantum field is confined between two walls it generates a dependence of the renormalized vacuum energy on the boundary conditions at the space between these walls. This dependence of the vacuum energy is the Casimir energy. The behaviour of this Casimir energy for a massive scalar field shows an exponential decay with the distance between the walls and the mass, but also has a coefficient which separates boundary conditions in two types depending on the strength of this decay[1]. In 2+1 dimensions there exists some theoretical work that supports a reparametrization of gauge fields in terms of massive scalar fields [2,3]. In this talk, we are going to compute numerically the Casimir energy for SU(2) gauge theory using lattice simulations, and compare the results with those of a massive scalar field for boundary conditions that belong to different types of the exponential decay. This should provide a robust test about the idea that the infrared behaviour of gauge theories follows an effective scalar field with a mass, which seems to be much lower than the glueball in some previous result on the literature[4,5].

[1] Asorey, M.; Iuliano, C.; Ezquerro, F. Casimir Energy in $(2 + 1)$ -Dimensional Field Theories. *Physics* 2024, 6, 613-628.

[2] Karabali, D. Kim, C.; Nair, V. Planar Yang-Mills theory: Hamiltonian, regulators and mass gap. 352 *Nuclear Physics B* 1998, 524, 661-694.

[3] Karabali, D.; Nair, V. On the origin of the mass gap for non-Abelian gauge theories in $(2+ 1)$ 354 dimensions. *Physics Letters B* 1996, 1, 141-147.

[4] Chernodub, M.N.; Goy, V.A.; Molochkov, A.V.; Nguyen, H.H. Casimir Effect in Yang-Mills 348 *Theory in D = 2 + 1*. *Physical Review Letters* 2018, 121, 191601.

[5] Karabali, D.; Nair, V.P. Casimir effect in $(2 + 1)$ -dimensional Yang-Mills theory as a probe of the magnetic mass. *Physical Review D* 2018, 98, 105009.

Symplectic realizations and Lie groupoids in Poisson Electrodynamics

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Abstract

Following the ideas at the basis of deformation quantization, Poisson manifolds can be interpreted as semiclassical limits of quantum spacetimes. Therefore, the departure point towards the construction of proper gauge theories on a quantum spacetime consists in understanding what could be its semiclassical counterpart and what are the differences with respect to standard Yang-Mills gauge theories. This is the rationale behind the recent interest in studying suitable models of gauge theories on Poisson manifolds. In particular, in this talk I will present some results concerning the interpretation of gauge symmetry and the involved geometrical structures in the case of Poisson electrodynamics, where the gauge structure is determined by the group $U(1)$. Firstly, one defines the gauge potentials of Poisson electrodynamics as sections of a symplectic realization of the spacetime manifold. Then, infinitesimal gauge transformations appear as a representation of the associated Lie algebroid acting on the symplectic realization. This is a generalization of the infinitesimal action of the gauge group of classical electrodynamics (addition of a gradient), this action being recovered in the limit of vanishing Poisson structure. Finite gauge transformations are obtained by integrating the sections of the Lie algebroid to a one-parameter group of bisections of the corresponding symplectic groupoid. These bisections determine a one-parameter group of transformations, whose action on the fields of the theory is realized in terms of an action groupoid. A covariant electromagnetic two-form is obtained, together with a dual two-form, invariant under gauge transformations. The duality appearing in the picture originates from the existence of a pair of orthogonal foliations of the symplectic realization, which produce dual quotient manifolds, one related with spacetime, the other with momenta.

A new approach to the theory of games: classical and quantum

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Abstract

A new approach to the theory of games, both classical and quantum, based on the notion of categories and groupoids is presented. The basic idea is to identify sequences of consistent actions of players with morphisms of a category. The objects of the category are a subset of the Cartesian product of the space of players and the space of configurations of the game. In this way the algebra of the game is defined as the algebra of the category and its properties can be studied using it and its representations. In particular, any game can be groupoidified by considering the groupoid generated by the category of the game. This allows to introduce in a natural way the state of the game as a positive definite function on the corresponding groupoid. This setting allows to treat on the same foot classical and quantum games. Quantum games will be characterised by incorporating the groupoids describing the quantum aspects of the theory into the definition of the space of configurations and actions. As an application the setting for non-local quantum games will be discussed.

1. John Von Neumann and Oskar Morgenstern. Theory of games and economic behavior, 2nd rev.1947.
2. Richard Cleve et al. Consequences and Limits of Nonlocal Strategies. 2010. arXiv: quant-ph/0404076 [quant-ph].
3. Luis Alberto Ibort Latre and Miguel A. Rodríguez. An introduction to groups, groupoids and their representations. CRC Press Taylor and Francis Group, 2020.
4. Cleve, R., Hoyer, P., Toner, B., & Watrous, J. (2004, June). Consequences and limits of nonlocal strategies. In Proceedings. 19th IEEE Annual Conference on Computational Complexity, 2004. (pp. 236-249). IEEE.
5. A. Ibort, M. Jimenez-Vazquez, A. Millán. "A new approach to the theory of classical and quantum games: categories and groupoids". In preparation (2024).

Categorical foundations of Quantum Field Theory: gauge invariance

1st author

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Abstract

Schwinger's picture of quantum mechanics inspired a categorical/groupoidal description of quantum mechanical systems that, in turn, provides a new approach to the foundations of quantum field theories. Such approach involves replacing the notion of the configuration fields of the theory by the notion of "histories". A history is a functor (that is a groupoid homomorphism) from a reference, test or probe groupoid to the quantum Schwinger groupoid of the system being described. For a significant class of probing groupoids the family of such histories becomes a C^* -category on which a Feynman-like path integral principle can be stated. This approach fills the bridge between Schwinger's quantum dynamical principle for quantum field theories and Feynman's Lagrangian path integral description. The particular instances of quantum mechanical systems with finite degrees of freedom and Dijkgraaf-Witten topological gauge theories will be used to illustrate the most salient points of the new set of ideas.

Implementing the Grover algorithm in homomorphic encryption schemes

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Abstract

Quantum homomorphic encryption (QHE) is an important cryptographic technology useful for delegated quantum computation. It allows a remote server to perform quantum computations on encrypted quantum data sent by a client, so that the server cannot obtain any information about the client's data. We apply QHE schemes suitable for circuits with a polynomial number of $T/T^\dagger$ -gates to Grover's algorithm, performing a simulation in Qiskit of a Grover circuit that contains 3 qubits. The $T/T^\dagger$ gate complexity of Grover's algorithm is also analysed in order to show that any Grover circuit can be evaluated homomorphically in an efficient manner. We discuss how to apply these QHE schemes to allow for the efficient homomorphic evaluation of any Grover circuit composed of n qubits using $n-2$ extra ancilla qubits. We also show how the homomorphic evaluation of the special case where there is only one marked item can be implemented using an algorithm that makes the decryption process more efficient compared to the standard Grover algorithm.

Tangent structures via coisotropic embeddings

1st author

Luca Schiavone Carlos III

Abstract

We discuss a construction based on the coisotropic embedding theorem that allows to construct non-degenerate Lagrangian theories from degenerate ones.

Kinematical groupoids and the description of elementary particles in curved spacetime

1st author

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Abstract

In standard accounts of QFT, the classification of fundamental particles in terms of mass and spin comes about as a result of Wigner's classification of the irreducible representations of the Poincaré group. Nevertheless, global Poincaré invariance only exists in flat Minkowski spacetime. It is then not clear how mass and spin as characterising quantum numbers of particles can be introduced in curved backgrounds. In this talk we show how by replacing the action of the Poincaré group by a suitable kinematical groupoid, which captures the local isometry invariance in curved backgrounds, one obtains irreducible representations characterized by the same quantum numbers of mass and spin. This result hinges on an appropriate generalisation of Mackey's imprimitivity theorem to the representation theory of groupoids.

Geometry of classical and quantum states

1st author

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Abstract

Classical and quantum finite-level systems are the subject of recent active investigation, especially because of the increasingly relevant role information theory is playing in modern technological development.

From the mathematical point of view, the structure of the space of states of a finite-level (classical or quantum) system may be probed using differential geometric techniques that do not "suffer" of all the functional-analytic subtleties typical of infinite dimensions, yet the emerging geometrical picture is both fascinating and rich enough to deserve a thorough study.

Accordingly, the purpose of this talk is to provide a bird-eye view on the geometry of classical and quantum states in finite dimensions, with a strong emphasis on those structures that arise from information-geometric considerations.

We will review the unique Riemannian geometry on probability simplexes according to ?encov's theorem, as well as its associated dual connections in the sense of information geometry. Then, we'll move on to discuss how these structures can be suitably generalized in the quantum case. Here, we lose the uniqueness typical of the classical case, and are flooded by infinite possibilities among which we'll try to navigate.

In particular, a recently discovered link between the possible quantum Riemannian geometries, the dualistic structures associated with the convex structure of quantum states, relative entropies, and the actions of suitable extensions of the unitary group that dress the manifold of faithful quantum states with different, but diffeomorphic, structures of homogeneous space will be discussed,

Finally, with the sincere hope of generating interest and stimulate discussions, a selection of open problems and future perspectives will be presented.

Hamilton-Jacobi's approach to precontrast functions in Information Geometry

1st author

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Abstract

The geometric content of a statistical manifold consists of a pseudo-Riemannian manifold equipped either with a pair of conjugate torsion-free affine connections or a fully symmetric 3-covariant tensor. These geometric objects can be encoded into a 2-point function called the contrast function. Recently, statistical manifolds admitting torsion (SMAT) have also been considered. They are pseudo-Riemannian manifolds equipped either with a pair of conjugate affine connections for which one of them is allowed to have torsion or a 3-covariant tensor invariant under a transposition of the entries. Even in this case, one can capture the geometrical structure through a function termed a precontrast function. The latter is no longer a 2-point function and the asymmetry of the input arguments manifests the lack of the dually-torsion-free nature of the induced connections. In this talk, I will review the construction of contrast functions starting from Lagrangian functions. Under appropriate regularity conditions, a complete solution of the Hamilton-Jacobi problem associated with a Lagrangian is a contrast function. Then, I will show how this approach can be extended to obtain precontrast functions.

From Normal probability distributions to the category of non-commutative probabilities

1st author

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Abstract

Normal distributions are an important example of statistical models. For them the covariance matrix of the sample mean and sample variance estimators is equal to the inverse of the so-called Fisher-Rao metric. Moreover, because of the Cramer-Rao inequality the inverse of this metric tensor provides a lower bound for the covariance matrix of any couple of unbiased estimators. The interesting connection between a statistical quantity (the covariance) and a geometrical one (the Fisher-Rao metric) encoded by the Cramer-Rao inequality also holds in more general statistical models. Therefore, it is natural to ask why is this geometry so central in statistics. The first to address this question was Ψ encov, who, in the light of category theory proved that the Fisher-Rao metric tensor is the only Riemannian metric tensor on probability simplexes, which is invariant under Markov maps implementing coarse-graining. A suitable reformulation of the Cramer-Rao inequality is also valid in the quantum context, where probability distributions are replaced by quantum states. In this case, however, the Fisher-Rao metric tensor is replaced by (one of) its quantum counterpart: the so-called Bures-Helstrom metric tensor. In analogy with the classical result and with an analogous categorical mindset, Ψ encov, together with Morozowa started to investigate the Riemannian geometries on invertible quantum states which do not increase under CPTP maps implementing coarse-graining. Nevertheless, it was Petz who, without adhering to any categorical setting, made a characterization of such geometries (in finite dimensions), proving that in the quantum case, uniqueness does not hold. In this talk, a reformulation of these problems will be presented. The natural framework of this reformulation turns out to be a suitable category of non-commutative probabilities, following Ψ encov's

original spirit. We will see how this category presents a perfect environment to discuss ?encov's and Petz's results, their unification, and their generalization to infinite dimensions.

Josephson Junctions: An open (modelling) problem?

1st author

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Abstract

Josephson Effect was predicted by Brian D. Josephson in a Nobel Prize awarded research in 1962. Since then the so-called Josephson Junctions have become a key component in technological developments. For instance, they can be used to build extremely sensible magnetometers or are part of the so-called superconducting quantum circuits. Despite its quantum origin, usual models are derived starting with the classical Current-voltage characteristic curves (IV curves) considering them as components of classical electrical circuits. A first quantization then leads to the Quantum Hamiltonians that are finally used to model them. I will present an overview of this procedure showing that it is not very satisfactory from a fundamental point of view and will point to possible alternatives for their description.

Quantum dynamics and quadratic forms: stability and control

1st author

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Abstract

According to Quantum Mechanics, the (pure) states of a quantum system are described by normalised elements of a complex separable Hilbert space, while their evolution is given by a t -dependent Hamiltonian, $H(t)$, through the Schrödinger equation. In the general case, this Hamiltonian is an unbounded t -dependent operator acting in an infinite dimensional Hilbert space and this introduces some problems for the existence of solutions of the Schrödinger equation. Basing on ideas developed by Jan Kisyński and Barry Simon, we will study the case on which the quadratic forms associated to the Hamiltonians have constant domain, reviewing sufficient conditions for existence of solutions of the Schrödinger equation and providing a new stability result for this solutions.

These results have applications in quantum control and will provide us with a common framework reviewing some unconventional quantum control problems such as controlling the quantum state of particle in a box by moving its walls, by manipulating its boundary conditions or even by means of delta-like interactions.

Ferroelectrics: from fundamental to applications (DFMC-GEFES) / *Materiales ferroeléctricos: desde aspectos fundamentales hasta aplicaciones (DFMC-GEFES)*

Organiser

Javier Junquera (Universidad de Cantabria) Jacobo Santamaria (UCM) Ignasi Fina (ICMAB)

Invited speakers

Jorge Iñiguez (Luxembourg Institute of Science and Technology) Laura Bégon-Lours (ETH Zürich) Suzanne Lancaster (NaMLab gGmbH) Sergei Prokhorenko (Luxembourg Institute of Science and Technology) Paula Vilarinho (University of Aveiro) Marti Checa (Oak Ridge National Laboratory)

Symposium abstract

Since over a century, ferroelectric materials have been the main topic of numerous research, both fundamental and applied. Its progressive understanding has been the origin of successive revolutionary experimental and theoretical advances, with an impact that goes far beyond the boundary of the ferroelectric community. In recent years, the stabilization of non-trivial topological phases, the observation of ferroelectricity in nanostructured phases based on hafnium dioxide (the material chosen by the semiconductor industry for its compatibility with silicon and its high dielectric constant), the manufacture of membranes based in oxide or the new 2D ferroelectric materials based on van der Waals interactions have revolutionized the field. All of these new phases are accompanied by exotic properties (negative capacitance, chirality, giant electrocaloric responses, magnetoelectricity and multiferroicity, etc.) that have had a great impact on diverse applications, ranging from actuators to electronic memories. This conference intends to discuss the most recent breakthroughs in this discipline, which never ceases to amaze

Desde hace algo más de un siglo, los materiales ferroeléctricos han sido el tema principal de numerosas investigaciones, tanto fundamentales como aplicadas. Su comprensión fundamental ha sido el origen de sucesivos y revolucionarios avances experimentales y teóricos, con un impacto que a menudo va mucho más allá del límite de la comunidad ferroeléctrica. En los últimos años la estabilización de fases topológicas no triviales, la observación de ferroelectricidad en fases nanoestructuradas basadas en dióxido de hafnio (el material elegido por la industria de semiconductores por su compatibilidad con silicio y su alta constante dieléctrica), la fabricación de membranas basadas en óxido o los nuevos materiales ferroeléctricos bidimensionales basados en interacciones van der Waals han revolucionado el campo. Todas estas nuevas fases vienen acompañadas de propiedades exóticas (capacidad negativa, quiralidad, respuestas electrocalóricas gigantes, magnetoelectricidad y multiferroicidad, etc) que han tenido un gran impacto en aplicaciones diversas, que van desde los actuadores a las memorias electrónicas. En este simposio se propone discutir los últimos avances en este campo que no deja de deparar sorpresas.

List of abstracts at the symposium

Unprecedented intrinsic properties of hafnia ferroelectrics

1st author

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Abstract

CMOS-compatible hafnia ferroelectrics hold great promise for the development of nano-devices that may take advantage of their permanent and switchable electric polarization, which has made them a focus of attention. But that is not all: surprisingly, these materials are proving to constitute a ferroelectric class of

their own, displaying many intrinsic behaviors that seem genuinely unprecedented and certainly lay outside the "standard model" of soft-mode ferroelectricity in perovskite oxides. In this talk I will present first-principles results to discuss and explain some of those intriguing intrinsic properties. I will focus on the piezoelectric response of hafnia ferroelectrics, which -- by comparison with the (trivial) behavior of a ferroelectric perovskite -- will allow me to illustrate many of their unique features: ambiguity regarding the sign of the polarization, (apparent) anomalous character of the piezoelectric effect, strategies to tune the sign of the piezoresponse and even cancel the effect while remaining ferroelectric. I will also show experimental evidence of some of these surprising properties. Time permitting, I will summarize other recent results of my group, e.g., on hafnia-based superlattices.

Work done in collaboration with Hugo Aramberri, Sangita Dutta, Binayak Mukherjee and Natalya S. Fedorova (Luxembourg Institute of Science and Technology), as well as the groups of Alexei Gruverman (U. Nebraska) and C. Dubourdieu (Helmholtz-Zentrum Berlin). Funded by the Luxembourg National Research Fund through Grant INTER/NWO/20/15079143/TRICOLOR.

Tuning of ferroelectric properties in doped ZrO₂

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Abstract

Zirconium oxide (ZrO₂) thin films show significant promise for diverse applications in energy storage, non-volatile memories, logic, and neuromorphic computing. Their compatibility with complementary metal-oxide-semiconductor (CMOS) technology, high dielectric constant and natural abundance makes them particularly attractive for large-scale utilization. Despite these advantages, ZrO₂ thin films have been understudied when compared to HfO₂ and hafnium-zirconium oxide (HZO), resulting in a limited understanding of their tunability and engineering. In bulk ZrO₂, the stable phases are the monoclinic (m) phase of space group P2₁/c and tetragonal (t) phase of space group P4₂/nmc. The FE behavior arises from the metastable polar o-phase of space group Pca2₁ and the polar rhombohedral (r) phase of space group R3m. Facilitating the stabilization of the polar phases is of utmost importance as they hold most of the interest in application, understanding the relative phase stability of this material is therefore a clear priority. The effect of doping has previously been studied both theoretically and experimentally for HfO₂ and HZO but not extensively for ZrO₂, showing great promise in allowing for the tuning of properties such as polarization, wake up, endurance, coercive field and switching times. Knowledge of the effects of doping on the relative phase stability, polarization, and piezoelectric response of ZrO₂ is still widely missing. In this study, employing density functional theory (DFT), we systematically investigate the impact of dopants on structural properties, relative phase stability, polarization, and the piezoelectric response of the polar orthorhombic phase of ZrO₂. Our analysis encompasses an extensive list of dopants and highlights the key candidates with exceptional potential for practical applications. Our findings add to and further solidify the current state of the art theoretical insight of the material and its potential for application.

Co/Hf_{0.5}Zr_{0.5}O₂ multiferroic heterostructures

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Abstract

Multiferroic materials encompass those with intertwined ferroic orders, such as the coexistence of ferroelectricity and ferromagnetism. Multiferroic magneto-electric materials, in particular, are seen as promising for energy-efficient spintronic applications, yet their scarcity and limited magnetoelectric coupling at low temperatures hinder practical use. Alternatively, multiferroic heterostructures offer promise, but many rely on ferroelectric perovskites, which struggle with CMOS integration and degrade with scaling down. However, the discovery in 2011 of robust ferroelectricity in doped HfO₂, compatible with CMOS, opens a compelling avenue. Despite the technological interest of ferroelectric HfO₂, there has been limited exploration into magnetoelectric effects between ferromagnetic electrodes and the ferroelectric HfO₂ films.

Here, a systematic characterization on the ferroelectric properties of epitaxial Hf_{0.5}Zr_{0.5}O₂ films deposited on buffered Si(001) with Co serving as the top electrodes will be presented. [1] The use of epitaxial films, which provide greater control over microstructural properties, facilitates understanding of the observed phenomena. Ferroelectric Hf_{0.5}Zr_{0.5}O₂ capacitors with Pt/Co top electrodes have similar high remanent polarization of about 25 $\mu\text{C}/\text{cm}^2$ and endurance of about 10^8 cycles as capacitors with the standard top Pt electrode. Remarkably, direct magneto-electric coupling effects are demonstrated when Pt/Co electrodes are used. Application of an external magnetic field does not change the remanent polarization, but it allows up to 40% modulation of the imprint field. Analyses of piezoelectric and flexoelectric effects suggest the latter is the most probable underlying mechanism for the observed magnetoelectric coupling. The reported magnetoelectric coupling phenomena could bring new functionalities in emerging electronic devices based on ferroelectric HfO₂.

[1] T. Zakusylo, A. Quintana, V. Lenzi, J. P. B. Silva, L. Marques, J. L. Ortolá Yano, J. Lyu, J. Sort, F. Sánchez, I. Fina Materials Horizons 2024, Advance Article.

Self-powered near-infrared photodetectors based on ferroelectric ZrO₂ thin films

1st author

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Abstract

Current research has demonstrated different types of self-powered photodetectors using standard semiconductors, hybrid inorganic-organic halide perovskites and inorganic perovskites, utilizing the photovoltaic effect, pyroelectric effect, piezoelectric effect, and synergic effects, such as the piezo-phototronic and pyro-phototronic effects [1,2]. Very recently, a novel type of self-powered photodetector exploring the coupling between the photovoltaic, the pyroelectric and the ferroelectric effects (i.e., ferro-pyro-phototronic effect) has attracted great interest, owing to the excellent photo current response achieved with this triple coupling [2,3]. The ferro-pyro-phototronic effect can therefore, be an important route towards improving the performance of self-powered photodetectors [2]. In this talk, we present recent results on self-powered photodetectors based on ferroelectric ZrO₂ thin films. Herein, the performance of the photodetectors is understood based on the ferro-pyro-phototronic effect where the polarization-dependent interfacial coupling can greatly influence the photodetector performance. The proposed device have strong responsivities and rise and fall times of only a few microseconds. The photodetector performance is optimized in terms of the chopper frequency, and poling voltage. Overall, our work demonstrates a very promising ultrafast photodetectors based on ferroelectric ZrO₂ thin films.

[1] S. Sahare, P. Ghoderao, M.K. Sharma, M. Solovan, R. Aepuru, M. Kumar, Y. Chan, M. Zió?ek, S.L. Lee, Z.H. Lin, Nano Energy, 107, p.108172 (2023).

[2] A.R. Jayakrishnan, J.P. Silva, K. Gwozdz, M.J. Gomes, R.L. Hoyer, J.L. MacManus-Driscoll, Nano Energy, p.108969 (2023).

[3] J.P. Silva, K. Gwozdz, L.S. Marques, M. Pereira, M.J. Gomes, J.L. MacManus-Driscoll, R.L. Hoyer, R.L., 2023. Carbon Energy, 5(6), p.e297. (2023).

Ferroelectric Synaptic Weights with Hafnia Superlattices

1st author

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Abstract

Expanding beyond traditional silicon, the integration of innovative materials into the back-end-of-line (BEOL) of CMOS circuits is essential for the advancement of Artificial Neural Networks accelerators. The hardware realization of synaptic weights necessitates the utilization of linear and reprogrammable resistive elements. Within ferroelectric tunnel junctions, resistance can be tailored by manipulating the arrangement of ferroelectric domains through electrical pulses. By partitioning ferroelectric HfZrO₄ into HfO₂-ZrO₂ superlattices, the crystallization temperature falls below the 400 °C threshold required for BEOL integration. A reduction in device footprint is accompanied by a notable increase in the maximum-to-minimum conductance ratio from 7 to 32. Operating from ultra-fast (20 ns) to biological (500 μs) timescales, the synaptic plasticity is extensively characterized. Dynamic hysteresis mode, spanning up to 10¹¹ switching cycles, reveals the coexistence of ferroelectric and non-ferroelectric phenomena, such as defect rearrangement. Temperature-dependent transport measurements conducted under the linear (Ohmic) regime corroborate these findings. Additionally, the integration of superlattices into CMOS BEOL facilitates multi-level resistive switching. Demonstrating 1T-1R operation, this advancement lays the groundwork for the hardware realization of synaptic weights, enabling in-memory neuromorphic computing.

Hf(1-x)Z(x)O₂ monolayers for nanosupercapacitors: a performance assessment study

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Abstract

It's been now more than a decade since the discovery of ferroelectricity in doped HfO₂ thin films [1]. Among all other dopants, it has been shown that zirconium allows the lowest annealing temperature to crystallize orthorhombic phase, responsible for ferroelectricity, in polycrystalline Hf_{1-x}Z_xO₂ (HZO) monolayers [2]. Decreasing the annealing temperature allows to grow CMOS compatible monolayers. Additionally, a broader range of doping to crystallize the ferroelectric (FE) phase is observed for zirconium and at high doping, HZO layers can become antiferroelectric (AFE) [3]. The performance and properties of Metal/Insulator/Metal (MIM) capacitors will be presented, where the insulator is constituted by different HZO FE or AFE monolayers, depending on the processing conditions. A specific focus on AFE ZrO₂ Energy Density Storage (ESD) in function of processing parameters (annealing temperature, monolayer thickness) will be presented. Our results show one of the highest, if not the highest, ESD ever reported so far of 125 mJ/cm³ for a ZrO₂ monolayer of 10.3 nm. However, the efficiency and endurance of the MIM stack has also to be optimized and a wake-up effect is also observed for ZrO₂ thin films, which is rarely observed for ZrO₂ layers. A trade-off between these functional properties can be deduced from the study, to further optimize and reach the desired properties for a commercial supercapacitor. Nevertheless, the monolayer performance is extremely encouraging for attaining high energy storage density in multilayer stacks of HZO.

[1] T. S. Böske, J. Müller, D. Bräuhäus, U. Schröder, U. Böttger, Appl Phys Lett. 99, 102903 (2011).

[2] J. Müller et al., Appl Phys Lett. 99, 112901 (2011).

[3] Park, M. H., Lee, Y. H., Kim, H. J., Kim, Y. J., Moon, T., Kim, K. D., Müller, J., Kersch, A., Schroeder, U., Mikolajick, T., & Hwang, C. S., Advanced Materials, 27(11), 1811-1831 (2015).

Low oxidation conditions in pulsed laser deposition enhance polarization without degradation of endurance and retention in Hf_{0.5}Zr_{0.5}O₂ films

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Abstract

Since 2011, the discovery of ferroelectric (FE) properties in HfO₂-based materials have great attention to memory applications such as random-access memory, field effect transistor, and ferroelectric tunnel junction due to compatibility with CMOS, ultralow deposition thickness (e.g., ~10 nm), low leakage current, and high retention (>ten years). Endurance is the main limitation of FE HfO₂ for its future use in commercial devices. Significant progress achieved in the past few years has permitted gaining endurance up to 10¹¹ cycles, which is promising but significantly less than that of perovskite materials (up to 10¹⁵ cycles) [1]. However, the FE HfO₂ epitaxial films exhibited significant fatigue, and although the devices remain operational after 10¹¹ cycles, the polarization is significantly reduced. The improvement of the reliability of HfO₂ is challenged by the polarization–endurance and endurance–retention dilemmas: one usually decreases when the other enhances. These dilemmas are ascribed to oxygen vacancies. The oxygen pressure in a pulsed laser deposition (PLD) process affects the number of oxygen vacancies and stabilizes the orthorhombic (FE) phase during HfO₂ growth. However, if the oxygen pressure is high enough to thermalize the PLD plasma, the crystallinity of the films also degrades. Recently, we introduced Ar during PLD process [2]. Films deposited under mixed Ar/O₂ atmosphere with high O₂ pressure have better endurance despite their slightly higher fatigue due to the much larger polarization in pristine state. Therefore, the introduction of Ar in the deposition process improves the polarization of Hf_{0.5}Zr_{0.5}O₂ films without causing additional degradation in endurance and retention, and thus it permits a significant enhancement of the reliability.

[1] J. Lyu, T. Song, I. Fina, F. Sánchez, *Nanoscale* 2020, 12, 11280.

[2] T. Song, R. Solanas, M. Qian, I. Fina, F. Sánchez, *J. Mater. Chem. C* 2022, 10, 1084

Impact of reliability in multilevel operation of ferroelectric devices

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Abstract

Ferroelectric devices based on Hf_{0.5}Zr_{0.5}O₂ hold great promise in non-volatile memories and in emerging computing paradigms including neuromorphic applications. The ability to store multiple states in a single device adds new functionalities and decreases cell size. However, such devices are known to suffer from reliability issues including imprint (a systematic shift in coercive voltage over time) and limited retention (polarization loss or relaxation). Since many emerging applications of such devices rely on multilevel behaviour, it is imperative to understand the impact of reliability issues on the switching kinetics of ferroelectric devices, on the reproducibility of multilevel switching schemes and on device operation in ‘realistic’ scenarios. Therefore, we looked at modifying switching kinetics measurements in order to understand the impact of common reliability issues on multilevel device operation. These measurements will not only help to understand the tolerance of multiple states on factors such as delay times, but will also inform which types of reliability issues need to be targeted in order to enable reproducible partial switching characteristics.

Dynamical topological states and excitations in ultrathin ferroelectrics

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Abstract

Polar topological phases in ultra-thin ferroelectrics span a plethora of fascinating atomic structures ranging from crystal-like arrangements of vortex tubes and hexagonal bubble lattices to glass-like polar labyrinths. On the fundamental level, the out-of-equilibrium formation of these phases was linked to the emergence of Turing patterns through the theory of phase separation kinetics. Moreover, polar topologies were shown to give rise to many unusual physical phenomena, such as inverse transitions, negative capacitance, and chiral symmetry breaking.

Here, we report our recent results pertaining to yet another intriguing facet of polar topologies – the dynamical states such as vortex tube and bubble liquids. Using the first-principles-based effective Hamiltonian simulations of ultrathin $\text{Pb}(\text{Zr}_{0.4}\text{Ti}_{0.6})\text{O}_3$ under residual depolarizing field, we will show that, in both cases, the collective dipole dynamics within the liquid phase is governed by soft off-center phonons. Such phonons can be described as propagating vortex waves that become gapless at the transition temperature, thereby mediating the continuous $\text{SU}(1)$ symmetry breaking. Furthermore, we will discuss the fundamental implications of these results, such as (1) the structure and topology of the order parameter space associated with various polar topological phases and (2) the relation of polar vortex topologies with spin spiral states, liquid crystals as well as quantum spin- $\frac{1}{2}$ particles. Finally, we will explore the coupling of vortex waves with THz range ac electric fields and the non-linear dynamical phenomena it entails.

This research is supported by the Vannevar Bush Faculty Fellowship Grant No. N00014-20-1-2834 from the Department of Defense.

[1] Dynamics of polar vortex crystallization, [Suyash Rijal, Yousra Nahas, Sergei Prokhorenko, Laurent Bellaiche, https://arxiv.org/abs/2302.07380 \(2023\)](https://arxiv.org/abs/2302.07380)

[2] Motion and teleportation of polar bubbles in low-dimensional ferroelectrics, S. Prokhorenko, Y. Nahas, V. Govinden, Q. Zhang, N. Valanoor, and L. Bellaiche. Nat. Commun. 15, 412 (2024)

Phase transitions and domain dynamics in $\text{PbTiO}_3/\text{SrTiO}_3$ superlattices

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Abstract

Nanostructured ferroelectrics display exotic multidomain configurations resulting from the reduced dimensionality. In fact, the past decade has witnessed dramatic progress related to various aspects of emergent topological polar textures in oxide nanostructures which can display vortices, skyrmions, merons, hopfions, among others under suitable mechanical or electric boundary conditions [Rev. Mod. Phys. 95, 025001 (2023)]. These particle-like objects lead to interesting functional properties such as negative capacitance [Nature 534, 524 (2016)], chirality [Proc. Natl. Acad. Sci. U.S.A. 115, 915 (2018)] or stochastic ultrafast dynamics [Phys. Rev. Lett. 132, 136801 (2024)].

Understanding and controlling such particle-like dynamics is crucial for their usage in nanoelectronic devices, akin to the meticulous control achieved with their magnetic counterparts [Nat. Nanotechnol. 8, 8579 (2013)].

In this talk, we shall explore different phase transitions predicted by second-principles calculations on one of the model systems in the field $\text{PbTiO}_3/\text{SrTiO}_3$ superlattices as a function of temperature, strain or ferroelectric/dielectric thickness [Phys. Rev. B. 105, L220103 (2022), arXiv:2401.13026]. Moreover, atomistic second-principles studies suggest that domain-walls in $\text{PbTiO}_3/\text{SrTiO}_3$ superlattices become spontaneously mobile upon heating, with the polar order melting in a liquid-like fashion and showing ultrafast dynamics. We shall show molecular dynamics simulations of this model system to study the unique features of this transformation. Most notably, we find that the multidomain state loses its translational and orientational orders at different temperatures, resembling the behavior of liquid crystals and yielding an intermediate hexatic-like phase. Our simulations reveal the mechanism responsible for the melting and allow us to characterize the stochastic dynamics in the hexatic-like phase: we find evidence that it is thermally activated, with domain reorientation rates that grow from tens of gigahertz to terahertz in a narrow temperature window allowing a control on the domain life and diffusion times [arXiv:2401.13026].

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Reversible optical control of polarization in epitaxial ferroelectric thin films

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Abstract

Light-matter interaction in ferroelectric materials forms the basis for light to be used as a non-invasive probe for the spontaneous polarization. In recent years, a shift in perspective has given rise to the question whether light could also be used to actively manipulate domain configurations or even switch the ferroelectric polarization. Realizing such an electric-field-less remote handle of the polarization holds the potential to drastically simplify state-of-the-art ferroelectric device architectures and coin entirely new ferroelectrics-based optoelectronic applications.

In this work[1], we demonstrate optical control of the ferroelectric polarization in epitaxial PZT-based heterostructures. In this prototypical ferroelectric model system, we track the dynamic response of the polarization under above-bandgap excitation by UV light in real time using optical second harmonic generation. In films with a single-domain configuration, we find that UV-light exposure induces a transient change of the spontaneous polarization that depends on its out-of-plane direction. We attribute this behavior to a modification of the charge-screening environment driven by the separation of photoexcited charge carriers in the built-in electric field of the Schottky junction formed with the bottom electrode. Taking advantage of this phenomenon in films with a pristine depolarized multi-domain configuration, we accomplish remanent optical poling into a single-domain configuration at room temperature. We further demonstrate the reversibility of this optical poling by subsequent thermal annealing. Hence, our work paves the way for the all-optical control of the spontaneous polarization in ferroelectric thin films.

[1] M.F. Sarott et al. *Adv. Mater.* 2312437 (2024)

Hidden Topology of Translational Boundaries in up-up-down-down-type Ferroic Systems

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Abstract

Material topology is nowadays attracting an increasing interest due to the promising novel functionalities it can produce. It is often assumed that translational boundaries in collinear up-up-down-down ferroic systems exhibit trivial topology. Here, we reveal the possibility of spiral-like noncollinearity at such translational boundaries. Taking YbMnO₃ as a model system exhibiting collinear up-up-down-down spin order and using an ab-initio-based 1D chain model, we show the possibility of topologically non-trivial translational boundaries. The latter can be split into two quasi-independent spin subchains, each showing a distinct spiral-like evolution of the spin with an associated winding number that can differ between the two chains. We propose an order parameter that allows the continuum-theory description of the internal structure of such translational boundaries. Based on the constructed continuum-theory model, we identify the key model parameters controlling the topology of the boundaries: the nearest-neighbour and the next-nearest-neighbour exchange interactions, as well as anisotropy and biquadratic nearest-neighbour interactions. We further discuss the interaction between various types of translational boundaries and their response to an external field.

Novel photocaloric effects in archetypal ferroelectrics for solid-state cooling applications

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Abstract

Solid-state cooling presents an energy-efficient and environmentally friendly alternative to traditional refrigeration technologies that rely on thermodynamic cycles involving greenhouse gases. However, conventional caloric effects face several challenges that impede their practical application in refrigeration devices. Firstly, operational temperature conditions must align closely with zero-field phase transition points; otherwise, the required driving fields become excessively large. But phase transitions occur infrequently near room temperature. Additionally, caloric effects typically exhibit strong temperature dependence and are sizeable only within relatively narrow temperature ranges. In this talk, I will show based on first-principles simulation methods that light-driven phase transitions in polar oxide perovskites have the potential to overcome such limitations. Specifically, for the prototypical ferroelectric KNbO₃ I will illustrate the existence of novel and giant photocaloric effects induced by light absorption ($\Delta S_{PC} \sim 100 \text{ J K}^{-1} \text{ kg}^{-1}$ and $\Delta T_{PC} \sim 10 \text{ K}$) across a vast temperature range of several hundred Kelvin, encompassing room temperature. These findings are expected to be generalizable to other materials exhibiting similar polar behavior.

On demand nanoengineering of topological ferroelectric structures

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Abstract

Ferroelectric materials present a nuanced polarization landscape, holding significant promise as tunable electronic components for advanced beyond binary high-density computing devices. Writing and reading multiple polarization states dynamically in an automated and fast manner is necessary to achieve that goal. In this work, we demonstrate the possibility of utilizing smart scan trajectories of a biased atomic force microscope probe to control in-plane ferroelectric polarization, generating on-demand topologically protected and frustrated ferroelectric states that display an in-plane center-divergent/convergent and flux-closure structure in Pb_{0.6}Sr_{0.4}TiO₃. Using correlative piezoresponse force and second harmonic generation microscopies we study the switching mechanism that drives the polarization dynamics and demonstrate how such structures are highly tunable via probe speed, sparsity, bias, chirality etc. Furthermore, phase field modelling corroborates the stability of such arrangements and provides additional understanding on the local polarization reorientation. Our findings provide a path towards using such patterns in neuromorphic circuits and device architectures based on complex domain structures with measurable functional properties.

Finite-temperature properties of antiferroelectric perovskite PbZrO₃ from second-principles

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Abstract

The prototypical antiferroelectric perovskite PbZrO₃ (PZO) has attracted considerable attention for its importance in technological applications and fundamental research. However, many fundamental aspects of PZO, particularly those related to large length and time scales and finite temperatures, remain not fully understood. Traditional first-principles methods are typically restricted to zero Kelvin and small length and time scales due to the heavy electronic self-consistent iterations. A promising solution to overcome these

limitations is the “second-principles” method, which is to construct a first-principles-based effective interatomic potential, integrating out the electronic degrees of freedom, so as to enable efficient simulations for relatively large systems at finite temperatures.

In this study, we investigate the finite-temperature properties of PZO through second-principles atomistic simulations. We developed a deep learning interatomic potential for PZO which successfully captures a large number of different phases. Using this model, we explored the phase transitions of PZO during heating and cooling. When heating up from different low-energy phases, i.e. *Pbam*/*Pnam*, *Ima2* and *R3c*, we find that the antiferroelectric *Pbam* is always favored before the system goes into the cubic phase. The phase transition temperature from *Pbam* to the cubic phase in the simulation is very close to the experimental one [$T_C \approx 480$ K (cal.), 505 K (exp)]. When cooling down from the cubic phase, we find that the system first goes into *Pbam* and then stays there, while global transitions to other competing phases are likely kinetically hindered; the ferroelectric *Ima2* structures only appear locally in the form of translational boundaries. Furthermore, in the temperature range where the antiferroelectric *Pbam* phase is thermodynamically stable, characteristic double polarization hysteresis loops of antiferroelectrics were obtained, along with the detailed elucidation of the atomistic process for the electric field induced transitions between nonpolar *Pbam* and polar *R3c* phases from the simulation.

TBA

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POSTER: Ferroelectric characterisation of the solid solution $\text{La}_{2-x}\text{Er}_x(\text{MoO}_4)_3$ ($x = 0.85, 1.15$)

Presenter

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Co-presenters

Christian Hernández Álvarez Universidad de La Laguna

Manuel Torres Betancort Universidad de La Laguna

Cristina González-Silgo Universidad de La Laguna

Abstract

The interest in controlling both ferroelectricity and luminescent properties in the family of rare earth molybdates, which crystallise in the $\text{Gd}_2(\text{MoO}_4)_3$ phase, has led to the synthesis of solid solutions where different rare earth atoms are substituted. This work focuses on studying the ferroelectric behaviour of the solid solution $\text{La}_{2-x}\text{Er}_x(\text{MoO}_4)_3$ as a function of x -concentration, by means of x-ray diffraction, dielectric spectroscopy, ferroelectric hysteresis cycling and optical emission spectroscopy (Fig.1). The results obtained show the improper ferroelectric character of several of the concentrations analysed ($x = 0.85, 1.15$), in line with other concentrations previously studied [1]; furthermore, a wide range of transition temperatures from 300 to 600 K is observed, where the magnitude of the real part of the complex relative dielectric permittivity presents very small values (< 60) and the maximum polarisation between 0.12 and 1.2 $\mu\text{C}/\text{cm}^2$.

Advanced nanolithography in condensed matter physics (DFMC-GEFES) / Nanolitografía avanzada en Física de la Materia Condensada (DFMC-GEFES)

Organiser

Soraya Sangiao Barral (U Zaragoza-INMA)

Enrique Díez Fernández (U Salamanca)

Invited speakers

Harald Plank (Institute of Electron Microscopy and Nanoanalysis, Graz University of Technology)

Symposium abstract

Nanolithography encompasses the set of techniques that allow us to define, structure and contact systems on a nanometric scale and, therefore, is a key element in Nanotechnology. Since 2009, there has been the Spanish Nanolithography Network, the Nanolito Network, which allows the coordination of the different scientific-technical infrastructures and research groups that exist today in Spain in the field of Nanolithography. This symposium will present the latest advances in the application of advanced Nanolithography techniques to condensed matter physics, thanks to a series of speakers who will cover the most relevant current areas.

La Nanolitografía engloba al conjunto de técnicas que nos permiten definir, estructurar y contactar sistemas a escala nanométrica y, por tanto, es un elemento clave en la Nanotecnología. Desde 2009 existe la Red Española de Nanolitografía, la Red Nanolito, que permite la coordinación de las diferentes infraestructuras científico-técnicas y de los grupos de investigación que existen hoy en día en España en el campo de la Nanolitografía. En este simposio se presentarán los últimos avances en la aplicación de técnicas de Nanolitografía avanzadas a la física de la materia condensada, gracias a una serie de ponentes que cubrirán las áreas actuales más relevantes.

List of abstracts at the symposium

3D nanoprinting via focused electron beams: principles, applications and frontiers

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Abstract

Over the past decade, additive direct-write manufacturing has emerged as a transformative force, now occupying a pivotal role in research and development thanks to its distinctive capabilities. While methods have progressed impressively to the microscale and even found utility in industrial settings, the challenges intensify as we venture into the meso- and nanoscale realms, where demands for resolution, spatial precision, predictability, and reliability escalate significantly. Among the limited pool of additive direct-write technologies suitable for nanoscale fabrication, focused electron beam induced deposition (FE BID) has witnessed remarkable strides in recent years. This technology bases on the precise, localized synthesis of nanostructures induced by a particle beam, utilizing surface-adsorbed precursor molecules introduced into the vacuum chamber via gas injection systems. Consequently, FE BID imposes minimal constraints on substrate materials (in terms of vacuum-/ beam-compatibility) and surface morphologies, rendering it a bona fide additive direct-write method. One of FE BID's distinguishing features is its capability to fabricate intricate, freestanding 3D nanostructures through controlled manipulation of the electron beam combined with defined pulse durations. This enables the attainment of individual feature sizes down to the sub-10 nm range in a predictable and reproducible manner. Moreover, with an expanding repertoire of precursor materials and enhanced software packages facilitating robust upfront design, 3D FE BID has ascended to the

status of a veritable 3D nano-printer, poised to spearhead advancements in direct-write additive manufacturing at the cutting edge. In this presentation, we embark on a journey through the most important fundamental principles of 3D FEBID, delving into recent advancements while placing particular emphasis on the current state of fabrication techniques and tuning capabilities within 3D-space. We explore the intricacies of meshed, closed, and mixed 3D designs and highlighting their challenges during fabrication with the ambition to push the boundaries of this technology. Additionally, we scrutinize the technical and physical constraints that govern 3D FEBID, offering insights into the various application pathways through an examination of both direct and multi-stage procedures. This discussion is complemented by an exploration of materials, dissecting their structural and chemical compositions to illustrate how their properties can be tailored to suit specific requirements. Moreover, we showcase a range of examples spanning diverse fields such as nano-optics, electronics, magnetics, advanced scanning nanoprobes, and sensing applications, illustrating the wide-ranging applicability of 3D FEBID. Finally, we cast our gaze towards the horizon, offering a glimpse into the future of this technology, identifying nascent avenues in materials, research areas, and technological developments that are poised to shape the landscape in unprecedented ways.

Growth of metallic nanopatterns by Focused Ion Beam (FIB) direct modification of condensed precursor layers and spin-coated organometallic thin films

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Abstract

Focused Ion Beam (FIB) is a very relevant technique to pattern materials down to the nanoscale, either through the local removal of material or through the change of physical properties produced by the ion beam. Moreover, in combination with precursors, the ion beam gives rise to the growth of nanomaterials, a technique known as Focused Ion Beam Induced Deposition (FIBID). Unfortunately, FIBID is a slow technique, which limits its applicability. Here, two strategies that improve the throughput of FIBID by a few orders of magnitude will be shown. The first one is based on the condensation of precursors delivered through a gas injection system onto a cooled substrate (Cryo-FIBID) [1, 2]. With this approach, W, Pt and Co based deposits have been grown and their electrical properties have been investigated, with Co deposits reaching the lowest resistivity and highest metallic content. The second strategy is based on the ion-induced dissociation of spin-coated organometallic thin films, in particular Palladium Acetate films, leading to structures with high Pd content that do not require post-processing steps to achieve metallic functionality [3]. A few applications of the micro- and nano-structures grown with both strategies will be shown.

[1] J. M. De Teresa et al., *Micromachines* 2019, 10, 799

[2] A. Salvador-Porroche et al., *Nanoscale Advances* 2021, 3, 5656

[3] A. Salvador-Porroche et al., ACS Appl. Mater. & Inter. 2022, 14, 28211

Advanced Fabrication for the Observation of Phonon Polaritons in Large-Scale Multilayer Hexagonal Boron Nitride

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Abstract

Polaritons in layered materials (LMs) are promising candidates for the controlled manipulation of light at the nanoscale [1,2]. In this study, we present the observation of phonon polaritons (PhPs) in wafer-scale multilayer hexagonal boron nitride (hBN) grown via chemical vapor deposition (CVD) [3]. While previous studies predominantly rely on micromechanically exfoliated hBN flakes, the scalability of synthesis methods, such as CVD growth, is imperative for industrial applications [4]. To evaluate whether CVD-grown wafer-scale multilayer hBN can support phonon polaritons, we designed and fabricated nanoribbons, as PhP resonators. Notably, we achieved the fabrication of arrays of nanoresonators over areas of tenths of micrometers. The precise control over fabrication across large material areas resulted in the production of PhP resonators with quality factors of approximately 50. Furthermore, through infrared nanoimaging, we visualized PhPs and measured their lifetimes at approximately 0.6 picoseconds, comparable to those of micromechanically exfoliated multilayer hBN. These findings pave the way for the utilization of PhP-based surface-enhanced infrared spectroscopy, enabling applications such as gas sensing and infrared photodetectors [5]. Moreover, the development of advanced nanofabrication techniques tailored to these materials stresses the impact of scalable synthesis methods on emerging technologies.

[1] D. N. Basov et al., Polaritons in van Der Waals Materials, Science 354, aag1992 (2016).

[2] T. Low et al., Polaritons in Layered Two-Dimensional Materials, Nat. Mater. 16, 182 (2017).

[3] E. Calandrini et al., Near- and Far-Field Observation of Phonon Polaritons in Wafer-Scale Multilayer Hexagonal Boron Nitride Prepared by Chemical Vapor Deposition, Adv. Mater. 2302045 (2023).

[4] X. Li et al., Large-Area Synthesis of High-Quality and Uniform Graphene Films on Copper Foils, Science 324, 1312 (2009).

[5] S. Castilla et al., Plasmonic Antenna Coupling to Hyperbolic Phonon-Polaritons for Sensitive and Fast Mid-Infrared Photodetection with Graphene, Nat. Commun. 11, 4872 (2020).

Reducing thermal conductivity of layered MoS₂ by nanopatterning

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Abstract

Efficient thermal management of electronic devices presents significant challenges due to their high power densities. This study examines how layered MoS₂ phononic crystals (PnCs) effectively regulate thermal conductivity (k) while minimizing the impact on electrical conductivity. By employing suspended MoS₂ PnCs, we achieve an exceptionally low k value of approximately 0.1 W/mK, surpassing the amorphous limit while preserving the crystalline structure. Molecular dynamic simulations, incorporating parameters such as film thickness, porosity, and temperature, provide further validation for these findings. Our analysis reveals that layered PnCs outperform Si and SiC PnCs with comparable periodicity by approximately 100-fold, attributed to the pronounced anisotropic k of layered materials. To demonstrate the practical efficacy of this approach, we develop suspended heat-routing structures engineered to confine and direct heat flow along predefined pathways within the PnCs. This investigation underscores the substantial potential of layered materials as directional heat spreaders, thermal insulators, and active components for thermoelectric devices, offering a promising solution for thermal management in nanoelectronics.

Hydrodynamic flow in graphene heterostructures

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Abstract

In most solids, electron transport is typically determined by sample geometry, electron-phonon interaction, and electron-impurity interaction, characterized by the inelastic mean free path (l_e). In such solids, electron-electron interactions, characterized by the elastic mean free path (l_{ee}), play a secondary role ($l_{ee} \gg l_e$). However, recent progress in high-quality materials have facilitated the exploration of electrical transport in the hydrodynamic regime, where increasing l_e makes elastic interactions more significant. In this regime, Coulomb interactions drives electron motion from independent particles to collective motion of a viscous "electron fluid."

Above a certain temperature, graphene encapsulated in hBN can exhibit large l_e , greater than l_{ee} , making it an ideal candidate for the study of the hydrodynamic regime. Viscous electron flowing in graphene exhibits exotic signatures such as superballistic conduction. To enhance these hydrodynamic effects, it is crucial to modify the geometry of the device, and so, we have fabricated different samples with different geometries, like nanoconstrictions, crenellated channels, Tesla valves and some others, designed to enhance hydrodynamic effects. We will show their electrical response as a function of temperature, carrier density and external magnetic field, finding for some of them scaling laws which help us discuss the different transport regimes. We support our findings with detailed simulations of the Boltzmann transport equation and have found an enhanced superballistic effect with a non-monotonic behaviour with the magnetic field. Our simulations provide the explanation for our experimental results contributing to a better understanding of hydrodynamic transport and superballistic conduction.

- [1] M. Polini *et al.* Viscous electron fluids, Phys. Today 73, 28 (2020).
- [2] G. Varnavides *et al.* Charge transport and hydrodynamics in materials, Nat. Rev. Mater. 8, 726 (2023).
- [3] Aydın Cem Keser *et al.* Geometric Control of Universal Hydrodynamic Flow in a Two-Dimensional Electron Fluid. Phys. Rev. X 11, 031030 (2021).

Combination of thermal scanning probe lithography and directed self-assembly of block copolymers for nanoelectronics

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Abstract

For the future semiconductor technology nodes (3 nm node and beyond) alternative or complementary lithography techniques to extreme UV Lithography will be needed to further increase resolution, reduce line edge roughness and improve alignment accuracy. We present our results on the combination of thermal scanning probe lithography (t-SPL) and contact hole shrink (CHS) by grapho-epitaxial directed self-assembly (DSA) of block co-polymers (BCP) for high alignment accuracy and high resolution patterning. t-SPL patterning is based on the local sublimation of a polymeric resist layer with the heated tip of a scanning probe microscope. As the same tip is used for patterning and imaging, t-SPL can deliver extremely high overlay alignment accuracy. CHS by DSA of BCP is a bottom-up lithography process with potential resolution below 10 nm. It is based in spin coating and annealing a block copolymer into cylindrical guiding patterns. After annealing, microphase separation of the two BCP blocks and selective removal of one of them, the diameter of the original guiding pattern can be reduced by around 70%. The high alignment

accuracy given by t-SPL with the improved pattern resolution provided by DSA can be used, for example, to contact a high density array of electrostatic gates for semiconductor qubits.

Nanoimprinted Conductive Nanotopographies for Cell-Instructive Electromechanical Stimulation

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Abstract

Conductive nano-topographies hold promise for enhancing cellular responses and enabling precise electrophysiological stimulation of neural cells. These nano-topographies, which include nanogratings or nanopillars, have been shown to provide a unique environment for Neural Stem Cells (NSCs), offering both mechanical and electrical cues that can influence their growth and differentiation. These cues, by imitating the inherent electrical and mechanical characteristics of neural tissue, have the potential to promote the differentiation of neural stem cells (NSCs) and facilitate the development of functional neural networks. Hence, these nanotopographical cues hold promise for nerve repair, regeneration, and the treatment of neurodegenerative diseases using cells.

In this context, we explored a novel process for creating electrically conductive nanotopographies in polystyrene carbon-nanotube surface-nanocomposite by nanoimprint lithography. The surface-nanocomposites were created by spin-coating suitable carbon-nanotubes dispersions over polystyrene films, reaching the electrical percolation threshold, followed by thermal nanoimprint of the relevant nanotopographic features. Microscopic and localised confocal Raman spectroscopy studies confirmed the presence of carbon nanotubes dispersed within the imprinted surface nanofeatures. This fabrication method maintains an acceptable level of optical transparency on the substrate.

Our findings demonstrate that electrically conductive nanostructured surfaces enhance the differentiation of cultured NSCs when compared to smooth controls. The NSCs displayed the ability to generate both neurons and supporting glial cells over the nanostructured topographies. Their coordinated movement along the nanostructured ridges facilitated enhanced electrical communication between cells, which plays a critical role in forming functional neural networks.

POSTER: Design and control of a 20 um Fresnel zone plate lens in silicon substrates using Electron-beam lithography

Presenter

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Abstract

X-ray microscopy is a widely employed technique in diverse fields such as biological research, materials science, forensic science, trace metal analysis and Cell Morphology and Physiology. In order to achieve high spatial resolution, enhance intensity, collimate beams and improve energy resolution, X-ray microscopy requires optical elements [1]. Fresnel Zone Plates (FZPs) offer an efficient approach that allows for significant material savings and compactness without sacrificing optical performance. These optical components may be used to focus and photograph X-ray photons as well as other types of particles, such as atoms and neutrons [2], we provide detailed insights into the fabrication process of a Fresnel zone plate featuring 100 distinct zones, a diameter of 20 μm and an outermost zone width of 50 nm. We have developed a robust approach leveraging Electron Beam Lithography (EBL) [3] for precise definition of micrometric structures, coupled with optimization of a chromium mask [4] to ensure successful fabrication of the FZP via cryo-etching (1a-b). To prevent a critical collapse of structures, we thoroughly examine all the steps of the developed methodology, paying particular attention to the various etching processes (1.c).

[1] Schmahl, G. (1983). X-ray microscopy. Nuclear Instruments and Methods in Physics Research, 208(1-3), 361–365.

[2] O. Carnal, M. Sigel, T. Sleator, H. Takuma, J. Mlynek. Imaging and focusing of atoms by a Fresnel Zone Plate, Phys. Rev. Lett. 67 (1991) 3231-3234.

[3] Tan, N., Zhang, X., Neo, D., Huang, R., Liu, K., & Kumar, A. (2021). A review of recent advances in fabrication of optical Fresnel lenses. Journal of Manufacturing Processes.

[4] Nguyen, V., Shkondin, E., Jensen, F., Hubner, J., Leussink, P., & Jansen, H. (2020). Ultrahigh aspect ratio etching of silicon in SF₆-O₂ plasma: The clear-oxidize-remove-etch (CORE) sequence and chromium mask. Journal of Vacuum Science & Technology A, 38(5).

Molecular biophysics (DFMC-GEFES) / Biofísica molecular (DFMC-GEFES)

Organiser

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Invited speakers

Felix Ritort (Universitat de Barcelona, Spain) Aitziber López Cortajarena (CICbiomaGUNE, Spain) Ismael Díez-Pérez (King's College London, UK) Edmund Leary (Imdea Nanociencia, Spain) Guilherme Vilhena (ICMM, Spain), Mercedes Hernando-Perez (Universidad Autónoma de Madrid, Spain)

Symposium abstract

Over the last decade, the research on molecular biophysics has flourished remarkably, encompassing a broad range of research topics. Amongst others, the two fields of charge transfer through biosystems and single-biomolecule manipulation through e.g., optical or magnetic tweezers stand out due to the significant interest they have sparked, enabling the understanding of biomolecular processes and their exploitation for biomedical applications. The primary objective of this symposium is to bridge these two productive yet non-interacting communities, in order to foster a mutually-beneficial collaboration between ideally complementary partners, thus further expanding the frontiers of research in biophysics.

Durante la última década, la investigación en biofísica molecular ha florecido notablemente, abarcando una amplia gama de temas de investigación. Entre otros, dos campos que destacan son la transferencia de carga a través de biosistemas y la manipulación de biomoléculas individuales mediante, por ejemplo, pinzas ópticas o magnéticas, que han generado amplio interés debido a su utilizzo en la comprensión de procesos biomoleculares y en su explotación para aplicaciones biomédicas. El objetivo principal de este simposio es unir a estas dos comunidades productivas pero no interconectadas, con el fin de fomentar una colaboración mutuamente beneficiosa entre socios idealmente complementarios, expandiendo así aún más las fronteras de la investigación en biofísica.

List of abstracts at the symposium

Unveiling the Physical Principles of Protein Nanocages: single molecule approach using AFM

1st author

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Abstract

Viruses are nanosized, genome-filled, protein containers with remarkable thermodynamic and physical properties. Virus capsid must fulfil important stability requirements. They must be able to disassemble, in a controlled manner, to release their genome into the host cell, at the right time and place to give rise to a productive infection [4]. Viral Capsids must be stable enough to withstand harmful environmental conditions to protect the viral genome [1-3]. To adapt to these conditions and complete their cycle, viruses have evolved by modifying their capsid to achieve greater stability and protect the genetic material. These changes are manifested in physical properties (elastic constant, surface charge density, electromechanical properties, etc.) [5-8].

Here, I will present the physical characterization of viruses using Atomic Force Microscopy (AFM) in a liquid environment to elucidate the interplay between mechanical properties, structure, and biological function. Understanding the physical properties of viral capsids is vital not only for comprehending their biological lifecycle but also for designing nanocontainers for applications in bionanotechnology and nanomedicine.

- [1] Carrasco. C et al., *PNAS*, 106, 5475-5480 (2009)
- [2] Hernando. E et al., *Virology*, 267, 299–309 (2000)
- [3] Moody. M.F, *Journal of Molecular Biology*, 293, 401-433 (1999)
- [4] Mateu, M. G., *Archives of Biochemistry and Biophysics* 531, 65-79 (2013)
- [5] Hernando-Pérez. M et al., *Small*, 8, 2366-2370 (2012)
- [6] Cartagena. A, *Nanoscale*, 5, 4729-4736 (2013)
- [7] Hernando-Pérez. M et al., *Nanoscale*, 7, 17289-17298 (2015)
- [8] Hernando-Pérez. M et al., *ACS Nano*, 13, 7842–7849 (2019)

Tuning the Dynamics of Life: One Chemical Moiety at a Time

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Abstract

Life is inherently a non-equilibrium process whereby “the jiggling and wiggling of atoms”, functional building blocks (nucleic-acids and proteins) realize complex tasks in a synchronized manner far exceeding the ones anticipated from their structure alone. In this talk, I have selected two examples that portray how bio-molecular vibrations can be harnessed in different biological processes. Firstly I will show how a single oxygen atom differentiating dsDNA from dsRNA can completely alter their unwinding dynamics (pivotal in DNA/cell replication). Then, I unveil how DNA sequence is not only a chemical code but also a physical one, thus capable regulating different biological processes. In the second part of the talk, I shall focus on electron-transport processes occurring in proteins – pivotal in several biological processes (photosynthesis, respiration, ...). In particular, I will show how single point mutations provide the means to finely regulate molecular vibrations of the protein matrix surrounding the active redox-active site, thus giving the means to control/regulate charge-transport processes at single-protein level. Overall, these results showcase how vibrations at the molecular level are inextricably connected to different biological functions and conversely how such processes may be tuned/regulated through carefully designed molecular substitutions.

Studying DNA-protein interactions with a custom-built AFM-TIRF

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Abstract

The use of Atomic force microscopy (AFM) led to the visualization of individual biological molecules like proteins and DNA. However, this scanning technique struggles to differentiate molecules with similar topography. On the other hand, fluorescence microscopy allows to add labels to molecules trading resolution. In this project, we describe the development of a custom combined AFM/TIRF microscope that can obtain high resolution AFM images of fluorescently tagged molecules.

This integration requires adapting the piezo stage to accommodate a high numerical aperture (NA) objective. This setup has a larger mechanical loop what makes high resolution challenging, so we implemented a separate piezoactuator attached to the cantilever for high-speed Z-axis control. This allows the main piezo stage to handle XY, offset, and tilt adjustments while the smaller actuator provides precise Z-axis movement. This setup enabled us, to acquire high resolution images of DNA molecules using amplitude modulation (AM) AFM.

We built a TIRF microscope that utilizes a 488 nm excitation laser and features two signal capturing cameras. An EMCCD camera captures fluorescence emission at 530 nm with a pixel size of 70 nm/px, offering diffraction-limited resolution of fluorophores. Additionally, a CMOS camera provides a wider field of view ($127 \times 102 \mu\text{m}^2$) for capturing non-fluorescent features. For correlating images from both microscopes, we initially used 100 nm Tetraspeck beads as fiducial markers. Recently, we've achieved higher precision by using 4 nm tall DNA origami structures labeled with Alexa-Fluor488 dyes or SYTOX intercalator. These DNA origami structures offer a valuable tool for precise image correlation in biological measurements.

Adsorption-driven deformation and footprints of the RBD proteins in SARS-CoV-2 variants on biological and inanimate surface

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Abstract

Computational Biophysics has provided a broad and deep understanding of molecular-scale phenomena, during the recent pandemics, the direct transmission of the SARS-CoV-2 has elucidated the mechanisms of infection for the different variants that contributed to the development of vaccines and therapies. However, respiratory viruses, carried through airborne microdroplets, frequently adhere to surfaces, including plastics and metals. Our understanding of the interactions between viruses and materials remains limited, particularly in scenarios involving polarizable surfaces. Here, we investigate the role of receptor-binding domain (RBD) mutations on the adsorption of SARS-CoV-2 to hydrophobic and hydrophilic surfaces employing molecular simulations. To contextualize our findings, we contrast the interactions on inanimate surfaces with those on native-biological interfaces, specifically the ACE2 receptor. Notably, we identify a twofold increase in structural deformations for the protein's receptor binding motif onto the inanimate surfaces, indicative of enhanced shock-absorbing mechanisms [1]. Furthermore, the distribution of amino acids (landing footprints) on the inanimate surface reveals a distinct regional asymmetry relative to the biological interface. Despite the H-bonds formed at the hydrophilic substrate, the simulations consistently show a higher number of contacts and interfacial area with the hydrophobic surface. In contrast, the adsorption of delta and omicron to hydrophilic surfaces was characterized by a distinctive hopping pattern. The novel shock-absorbing mechanisms identified in the virus adsorption on inanimate surfaces could lead to current experimental efforts in the design of virucidal surfaces and sensors.

[1] A. Bosch, H. V. Guzmán, R. Pérez, (2024). Adsorption-driven deformation and landing-footprints of the RBD proteins in SARS-CoV-2 variants onto biological and inanimate surfaces.

(<https://doi.org/10.1101/2024.01.15.575706>) (Submitted)

[2] S. Poblete et al. 2021. ACS omega, 6(48), pp.32823-32831.

Single-Protein Electronics

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Abstract

Bioelectronics is a rapidly evolving field moving towards designing nanoscale electronic platforms that allow *in vivo* sensing, fuel cell powering and chemical biosynthesis. Such devices typically require interfacing a complex biomolecular moiety as the active component to an electronic platform for signal transduction and/or electron source wiring. Inevitably, a true systematic design goes through a bottom-up understanding of the structurally related electrical signatures of such hybrid biomolecular circuits, which will ultimately lead us to tailor its electrical properties and exploit them as high performance bioelectronic devices with a wide variety of applications in organic electronics, sensing, biomanufacturing, *etc.*

In this contribution, we will present our latest efforts on understanding and control charge transport in a single-protein junction. Our approach relies on trapping individual redox proteins in a tunneling junction under electrochemical control to characterize their main electrical signatures. The method can capture very fine details of the charge transport mechanisms across proteins in an aqueous environment. Our results suggest that the transport mechanism through the protein backbone can be switched upon quenching of particular motions in the protein structure via surface mutations. We then compare the above redox protein model to a natural multiheme molecular wire. Multiheme proteins have been recently discovered as the building blocks in highly conducting pili and transmembrane structures of certain species of the so called electrical bacteria. We have trapped individual small tetraheme proteins (STC) in our tunnelling gap and measured conductance. STC constitutes a well-known repeating arrangement of *heme* cofactors along larger multiheme complex structures. Our first results suggest a single STC unit can transport electrons via efficient electron tunnelling process along the ~4 nm long protein axis with very shallow electron decay constant. We believe these results contribute to the observed long-range charge transport behaviour observed in these multiheme-based molecular wires.

Chiral discrimination in biological systems induced by spin-dependent van der Waals interactions.

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Abstract

Space inversion symmetry in chiral molecules is broken. As a consequence, the electric and magnetic polarizabilities are coupled. We analyze the influence of this symmetry breaking in determining a chiral-discrimination mechanism mediated by spin-dependent van der Waals (vdW) interactions, arising from fluctuations on the magnetic moment of the molecule analogous to the electric dipole fluctuations responsible for the conventional form of vdW forces. This mechanism can be understood in terms of the Chiral-Induced Spin Selectivity (CISS) effect, which requires the inclusion of spin-orbit interaction (SOI). The CISS-mechanism is determined by a magnetic molecular response to electron transport in a chiral potential even in the absence of

external magnetic fields. An alternative explanation, which does not require the inclusion of SOI, is based in exchange interactions associated with the antisymmetric character of the many-electron wavefunction. In either case, the emerging feature is a chiral-discrimination term that is added to the conventional London expression for vdW forces, which changes sign depending on whether the interaction between two chiral molecules, with two enantiomers, D and L, occurs either for the (DD) or (LL) pairs or for the (DL) one. This apparently simple result has profound consequences for biological system because it provides a way for long-distance chiral recognition based on vdW interactions. In a recent publication¹, we have successfully tested our model in providing an interpretation for chiral discrimination observed through Atomic Force Microscopy experiments. The potential applications of these results to the pharmacological industry, and in the area of quantum molecular sensors, are also discussed.

(1) Y. Kapon, Q. Zhu, S. Yochelis, R. Naaman, R. Gutierrez, G. Cuniberti, Y. Paltiel, V. Mujica; Probing chiral discrimination in biological systems using atomic force microscopy: The role of van der Waals and exchange interactions. J. Chem. Phys. 14 December 2023; 159 (22): 224702. <https://doi.org/10.1063/5.0171742>

Efficient electron hopping transport through Azurin-based junctions

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Abstract

Proteins have been proven to be promising candidates for molecular electronics, showing in some cases much higher conductance than one would naively expect from their size. In particular, the blue-copper azurin extracted from *Pseudomonas aeruginosa* has been the subject of many experimental studies. The exact nature of the transport mechanism, however, is still under debate [1-7].

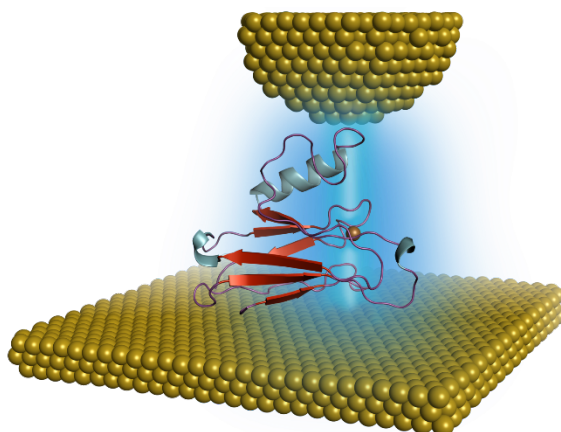


Fig 1. Geometry of a frame of the MD simulations of the gold-azurin-gold junction. Blue light represents the electron transport process of hopping through the copper atom. This illustration will appear as the Front Cover of the next issue of the J Phys Chem Lett journal.

In this work, we have conducted theoretical simulations to shed light on this issue. We found that single-site hopping can lead to either higher or lower current values compared to fully coherent transport. This depends on the structural details of the junctions as well as the alignment of the protein orbitals. Moreover, we show how the asymmetry of the IV-curves can be affected by the position of the tip in the junction and that, under specific conditions, such a hopping mechanism is consistent with a low temperature dependence of the current. Finally, we show that increasing the number of hopping sites leads to higher hopping currents [8].

- [1] Ruiz, M. P.; et al. *J. Am. Chem. Soc.*, 2017, 139, 15337–15346
- [2] Romero-Muñiz, C.; et al. *Phys. Chem. Chem. Phys.*, 2018, 20, 30392–30402
- [3] Romero-Muñiz, C.; et al. *Biomolecules*, 2019, 9, 506
- [4] Romero-Muñiz, C.; et al. *J. Phys. Chem. C*, 2021, 125, 1693–1702
- [5] Romero-Muñiz, C.; et al. *Appl. Sci.*, 2021, 11, 3732
- [6] Romero-Muñiz, C.; et al. *Front. Phys.*, 2022, 10
- [7] Papp, E.; et al. *J. Phys. Chem. B*, 2023, 127, 1728–1734
- [8] Roldán-Piñero, C.; et al. *J. Phys. Chem. Lett.*, 2023, 14, 11242–11249

Ionic Conductivity in Engineered Protein Thin Films

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Abstract

Protein-based conductive materials are promising for next-generation bioelectronics due to their versatility, biocompatibility, and biodegradability. Protein films composed of engineered consensus tetratricopeptide repeat (CTPR)[1] – proteins with a high content of negatively charged amino acids – have been demonstrated to be ionic conductors [2], with the dominant mechanism being protonic conduction. Proton transport within proteins is of interest for designing biocompatible energy storage devices or intelligent devices such as biosensors; raising the interest on improving protein film conductivities that can make them suitable for applications. In this work, we present an electrical characterization of thin films (~ 100-200 nm thickness) prepared using engineered CTPR protein variants modified by different rates of glutamic acid substitution. From impedance spectroscopy measurements of CTPR films drop-casted on interdigitated electrodes, we find an increase of ionic conductivity with increasing the substitution rate, which suggests an increase in protonic carrier concentration. Additionally, we investigate the impact of NaCl doping on the ionic transport of the films, finding also an improved conduction performance of engineered variants. Finally, we explore the variations of the mechanical properties of the films with the amino acid substitution. Our results suggest that engineered proteins, such as modified CTPR scaffolds, can generate appropriate materials for bioelectronics applications.

[1] Kajander T, Cortajarena A L, Main E R G, Mochrie S G J and Regan L 2005 A New Folding Paradigm for Repeat Proteins *J. Am. Chem. Soc.* 127 10188–90

[2] Carter N A and Grove T Z 2018 Protein Self-Assemblies That Can Generate, Hold, and Discharge Electric Potential in Response to Changes in Relative Humidity *J. Am. Chem. Soc.* 140 7144–51

Simulating Proton Transport through Peptide Nanotubes

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Abstract

Peptide nanotubes consist of cyclic peptides piled on top of each other and held together by hydrogen bonds, making them similar to carbon nanotubes in morphology. These materials are interesting from both a fundamental point of view, as they serve as a testing ground to study proton transport in more complex biomolecular systems, and from a technological perspective, as they are promising proton conducting materials for the development of fuel cells, batteries, sensors, and other advanced technologies. However, proton transport in peptide nanotubes is far from being well understood. Recent experiments on cyclic peptides based on phenylalanine and functionalized with either lysine, arginine, or histidine [1, 2] have shown an order-of-magnitude higher proton conductivity in lysine-containing nanotubes, which also varies drastically with the system's hydration level and counter-ion doping. Inspired by these results, we carried out molecular dynamics simulations to study the structure and dynamics of these systems. We find that peptides nanotubes can form bundles with channels between them, where the water molecules and counter-ions can enter and form a rich and dynamic structure of hydrogen bonds with the lysine sidechains. This structure appears to be a

viable candidate for mediating proton transport through a Grotthuss-like mechanism. We have also analyzed the influence of varying the water content and counter-ion doping on this network. Finally, preliminary QM-MM simulations have suggested that classical potentials may not accurately describe the hydrogen bonds within the peptide nanotubes, which may be an important information to consider when attempting to understand proton transport through these systems.

- [1] O. Silberbush, M. Engel, I. Sivron, S. Roy, and N. Ashkenasy, J. Phys. Chem. B, 123, 46, 9882-9888 (2019)
[2] S. Roy, L. Zheng, O. Silberbush, M. Engel, Y. Atsmon-Raz, Y. Miller, A. Migliore, D. N. Beratan, and Nurit Ashkenasy, J. Phys. Chem. B, 125, 46, 12741-12752 (2021)

Universal Cold RNA Phase Transitions

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Abstract

RNA's diversity of structures and functions has impacted all life forms since *primordia*. RNA energy landscapes are rough with many local minima that lead to glassy behavior. Using calorimetric force spectroscopy, we investigate RNA folding landscapes in previously unexplored low-temperature conditions. We find that Watson-Crick RNA hairpins, the most basic secondary structure elements, misfold into compact tertiary folds below a glassy transition temperature $T_G \sim 20^\circ\text{C}$ where the RNA heat capacity abruptly changes. We hypothesize that RNA cold misfolding is a general phenomenon driven by the ubiquity of RNA-water interactions, which leads to universal RNA phase transitions below T_G , such as maximum stability at $T_S \sim 5^\circ\text{C}$ where water density is maximum, and cold denaturation at $T_C \sim -50^\circ\text{C}$. RNA in the cold opens a paradigm for unexplored biochemistry with novel functionalities at subfreezing temperatures.

Tuning the Assembly of Proteins and Peptides in Lipid Bilayers

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Abstract

Interactions between peptides and lipids play a pivotal role in orchestrating intricate processes within cellular membranes, such as cell signaling and viral fusion. They are fundamentally important for maintaining membrane integrity and regulating membrane protein functions. Moreover, short peptides have sparked considerable interest in recent years due to their applications in nanomedical innovations propitiated by their ability to interact with biological systems [1]. Understanding these processes requires studying these interactions at a molecular level, which is empowered by computational tools, such as Molecular Dynamics (MD) simulations. While all-atom (AA) MD simulations can accurately model peptide conformation, they become computationally expensive when studying large systems and long timescales. Instead, coarse-grained (CG) models allow for the necessary conditions to model these systems. However, accurately reproducing the behavior of these peptides requires identifying their most stable conformations using AA-MD, which are then

mapped into the CG model. We employ the MARTINI CG force field, developed to simulate the behavior of lipid membranes and proteins [2, 3] to comprehend the mechanisms underlying the interactions and structural assemblies of peptides on lipid membranes. Our aim is to use this understanding to engineer proteins and peptides that assemble into novel configurations, thereby designing membrane complexes to improve existing drug delivery systems.

- [1] K. Desale, et al., Biomater. Sci. 9 (2021) 4: 1153-1188.
- [2] S. J. Marrink, et al., The Journal of Physical Chemistry B 111 (2007) 27: 7812-7824.
- [3] L. Monticelli, et al., Journal of Chemical Theory and Computation 4 (2008) 5: 819-834.

Molecular biophysics of double-strand DNA break repair

1st author

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Abstract

The viability of all organisms relies on multiple DNA transactions that take place within the cell nucleus, including the repair and maintenance of genetic material. These essential DNA manipulations are carried out by proteins acting as genuine nano-machines, efficiently cutting, pasting, or copying fragments of DNA. Among these processes, those performed to fix any potential damage produced to the DNA are crucial. A wide variety of DNA damage types have been described, yet double-strand breaks (DSBs) stand out as one of the most detrimental DNA lesions. Two primary pathways, Homologous Recombination (HR) and Non-Homologous End Joining (NHEJ), are responsible for the repair of DSBs. Both pathways involve intricate DNA transactions catalysed by proteins that sequentially or cooperatively work to fix the damage. Single-molecule methods enable the visualization of these complex transactions and the characterisation of protein:DNA intermediates involved in DNA repair. In this talk, I will describe how magnetic and optical tweezers, two single-molecule techniques, can be employed to monitor and observe protein machines at work, ultimately enhancing our understanding of the complex DNA transactions involved in the repair pathways of double-strand breaks.

Mechanisms of DNA-mediated allostery

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Abstract

DNA allostery refers to the indirect interaction between proteins bound at distant binding sites along the DNA. In contrast to the existing paradigm of DNA being a passive sequence, the double helix acts as a mediator for the propagation of mechanical signals from one binding site to the other. This induces cooperative (or antagonistic) binding of pairs of proteins which is relevant for the regulation of gene expression. However, hitherto DNA allostery has remained poorly understood. We discuss here a mechanical model of DNA/protein interactions which predicts three different mechanisms of DNA mediated allostery. Two of these mechanisms are enthalpy-driven, while a third is mediated through entropy. We compare predictions of our model to recent experiments of DNA allostery and identify which type of allostery fits the data best.

Ballistic Conductance through Porphyrin Nanoribbons

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Abstract

The search for long molecular wires that can transport charge with maximum efficiency over many nanometers has driven molecular electronics since its inception. Single-molecule conductance normally decays with length and is typically far below the theoretical limit of G_0 ($77.5 \text{ } \mu\text{S}$). Here, I will show that the conductances of a family of edge-fused porphyrin ribbons (lengths 1–7 nm) display remarkable behavior. The low-bias conductance is high across the whole series. Charging the molecules in situ results in a dramatic realignment of the frontier orbitals, increasing the conductance to $1 G_0$ (corresponding to a current of $20 \text{ } \mu\text{A}$). This behavior is most pronounced in the longer molecules due to their smaller HOMO–LUMO gaps. The conductance-voltage traces frequently exhibit peaks at zero bias, showing that a molecular energy level is in resonance with the Fermi level. This work lays the foundations for long, perfectly transmissive, molecular wires with technological potential.

Backbone charge-transfer pathways in micro-solvated double-stranded dry DNA

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Abstract

We show that dry-DNA single-molecule charge transport over distances of tens of nanometers is influenced by a high degree of dynamical disorder involving the bases. Such disorder destroys π -stacking and weakens base-mediated transport channels. In addition, the low hydration environment underscreens the coulombic interactions between negatively charged phosphate groups, lowering the phosphate group ionization potentials. Under these circumstances, the dominant charge-transport pathways can be phosphate-mediated. Such pathways explain recent single-molecule experiments that compare currents in intact and nicked 100 base-pair dry DNA structures. More generally, our simulations show that the standard paradigm of base-mediated charge transport in DNA is not universally valid under conditions of very-low hydration and very-long distance. In such conditions, even the nature of dynamic disorder is dependent on the DNA sequence because the low-hydration environment cannot prevent transient unfolding of DNA and the unfolding depends on the DNA sequence.

Engineering protein-based biomolecular materials and applications

1st author

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Abstract

Ordered protein-based biomaterials are highly desirable for a wide range of applications including templating, coating, sensing, bioelectronics, catalysis, and biomedicine. This has recently spurred the development, among others, of novel self-assembled materials and supramolecular nanostructures based on biomolecules. However, de novo design of protein-based materials is labour-intensive, and these materials are primarily designed as support scaffolds, as the entirety of the designed structure is required for the maintenance of structural integrity. In contrast, during protein crystallization, proteins naturally establish contacts with their

neighbouring protein units, creating macroscopic three-dimension scaffolds, i.e. crystals. We have explored strategies that rely on rational design of protein self-assembly and the re-engineering interactions within innate protein-protein contacts in crystalline lattices. On one hand, we demonstrate the potential to generate diverse crystalline protein frameworks by tuning the innate metal coordination preferences, guiding protein assembly for engineered consensus tetratricopeptide repeat (CTPR) proteins.[1] On the other hand, we have developed strategies to create ordered protein-based biomaterials by re-engineering protein-protein interactions that maintain the crystalline lattices, and by interfacing proteins with other self-assembly elements such as amyloid-derived peptides. Through these methods, we direct the assembly of proteins into structured thin films, 2D monolayers, or 3D tubular architectures.[2] Overall, the rational engineering of protein-based materials offers a promising approach for biomolecular materials with defined structural and functional properties. We present selected applications of these materials in the fields of bioelectronics,[3,4] and biomedicine.

[1] Liutkus, A...., Cortajarena, A,L., Protein Science (2024), in press.

[2] Sanchez-deAlcazar, D...., Cortajarena, A,L, Nanoscale Adv. (2019) 1: 3980-3991.

[3] Dominguez-Alfaro, A...., Cortajarena, A,L., Small (2022): 2307536

[4] Mejias, SH...., Cortajarena, A,L, Nanoscale (2021) 13: 6772-6779.

Puncturing lipid membranes with DNA nanopores

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Abstract

DNA nanopores appear to be a plausible alternative to the use of transmembraneproteins in the context of stochastic detection. In this method, tiny changes in the conductance provide information on the size of any analyte going across the lumen. In this paper, we investigate the dependence of insertion capabilities on the electrostatic properties of the nanopore and show that permanent electric dipoles considerably increase puncturing capabilities. We also investigate the possibility to trigger conformational changes with a single short oligonucleotide in a detectable way.

POSTER: Electrical Characterization of Tryptophan-Substituted Peptides Assemblies

Presenter

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Abstract

Bioelectronic materials, bridge biological and electronic systems, offering transformative potential in diverse applications ranging from biotechnology to biomedical devices. Proteins and peptides, with their inherent biocompatibility and self-assembly capabilities, have emerged as promising candidates for constructing bioelectronic interfaces. Peptide nanostructures offer a platform for precise engineering of electronic functionalities at the nanoscale. In this context, the integration of aromatic amino acids, such as tryptophan, can increase π -stacking interactions within peptides, thereby influencing their electronic properties.

In this study, we explored the self-assembly capabilities of different tryptophan-substituted peptides. We performed an electrical characterization under vacuum and ambient conditions. Our findings suggest that the selective inclusion of tryptophan residues in the peptide sequences resulted in enhanced interactions, which in turn yield substantial changes to their electrical properties.



New spin textures in magnetism (DFMC-GEFES) / Nuevas texturas de espín en magnetismo (DFMC-GEFES)

Organiser

Sandra Ruiz Gómez (Max Planck Institute for Chemical Physics of Solids, Dresden), Lucas Pérez García (UCM - IMDEA Nanociencia)

Invited speakers

Lucia Aballe (ALBA Synchrotron, Spain) and Aurelio Hierro (Universidad de Oviedo, Spain)

Symposium abstract

In recent years, the progress of nanofabrication techniques, together with the development of novel magnetic microscopies, have made it possible to both stabilize and observe new magnetic spin textures such as skyrmions, new types of magnetic walls or magnetic singularities. These new spin textures are not only interesting from a fundamental point of view, but they also have unique physical properties, such as topological protection, robustness under external magnetic fields, high mobility and speed or multifunctionality. These properties make them a crucial element in developing new devices for various applications, including medical technology and information and communication technologies. This symposium aims to gather the latest advancements in the field, encompassing fabrication and magnetic characterization techniques, as well as theoretical and experimental findings focused on their physical properties and potential applications. The symposium will focus on the following topics: a) Synthesis of 3D-nanomaterials. b) Magnetic microscopy for the study of spin textures. c) 3D and curvilinear nanomagnetism. d) Magnetization dynamics of domain walls in cylindrical systems. e) Dynamics of skyrmions and other spin textures. f) Spin textures in ferri and antiferromagnetic materials.

En los últimos años, el progreso de las técnicas de nanofabricación junto con el desarrollo de estrategias para realizar microscopía magnética tridimensional, han permitido tanto estabilizar como observar nuevas texturas de espín magnéticas tales como, skyrmions, nuevos tipos de paredes magnéticas o singularidades magnéticas. Estas nuevas texturas de espín, no solo resultan ser interesantes desde el punto de vista fundamental, sino que las nuevas propiedades físicas que presentan como la estabilidad frente a la aplicación de campos magnéticos, o la posibilidad de desplazarse a altas velocidades, hacen que sean un elemento clave en el desarrollo de nuevos dispositivos para aplicaciones que abarcan desde la tecnología médica hasta las nuevas tecnologías de la información y las comunicaciones. Este simposio pretende recoger los principales avances en el campo, incluyendo desde las técnicas de fabricación y caracterización magnética, que permiten la estabilización de estas estructuras, así como, resultados teóricos y experimentales centrados en sus propiedades físicas y sus posibles aplicaciones. En particular, el simposio abordará los siguientes temas: a) Fabricación de nanomateriales tridimensionales. b) Técnicas de microscopía magnética para el estudio de texturas de espín. c) Nanomagnetismo en sistemas tridimensionales y curvilíneos. d) Dinámica de paredes de dominio magnético en sistemas cilíndricos. e) Dinámica de skyrmions y otras texturas de espín. f) Texturas de espín en materiales ferri y antiferromagnéticos.

List of abstracts at the symposium

X-ray imaging of magnetic textures

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Abstract

Thanks to its elemental and orbital specificity, X-ray magnetic dichroism has become the reference technique for advanced magnetic characterization of materials. It is particularly well suited when extremely high sensitivity is required such as in the case of very diluted systems, ultrathin layers or nanostructures.

Microscopies using x-ray magnetic dichroism enable mapping simultaneously the chemistry and the domain landscape of magnetic nanostructures, films and surfaces with resolutions down to a few tens of nanometers and even below 10 nm in ptychographic approaches.

I will give an introduction to x-ray based magnetic imaging and an overview of the different experimental approaches. The strengths and limits of different methods will be highlighted, with particular emphasis on those available at the ALBA Synchrotron Light Facility, namely x-ray photoemission electron microscopy and transmission soft x-ray microscopy.

X-ray photoemission electron microscopy as available at the CIRCE beamline is a surface sensitive technique. It permits imaging magnetic nanostructures with sub-nanometer thickness and even fully compensated synthetic antiferromagnets. The available functional sample environments allow in situ experiments ranging from high temperatures to high frequency electric sample excitations. Transmission x-ray microscopy with soft x-rays as done at beamline MISTRAL on the other hand is a bulk-like method for thin samples. It is ideal for tomography and for imaging free-standing nano and microstructures, and is insensitive to applied magnetic and electric fields.

Examples from a variety of experiments and imaging modes will be presented in order to illustrate the possibilities offered by these instruments, open to external users through regular competitive calls.

Imaging of magnetoacoustic waves in ferromagnetic materials

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Abstract

Magnetoacoustic waves (MAWs) are joint magnetization and acoustic excitations in ferromagnetic thin films. The subject is gaining interest because acoustic generation of magnetization waves is energy efficient and uses well-established fabrication processes. Surface acoustic waves (SAWs) provide an efficient coupling between strain and magnetization, which makes it an attractive option to generate and

manipulate MAWs. The transformation of strain into magnetization is done through the magnetoelastic effect, which needs a magnetostrictive ferromagnetic material.

Direct imaging using X-ray Photoemission electron microscopy (XPEEM) together with X-ray magnetic circular dichroism (XMCD) allow for dynamic spin texture imaging, giving a complete picture of the behavior of MAWs compared to indirect measurements such as, acoustic ferromagnetic resonance. These techniques not only provide qualitative information but can also be used to quantifying MAWs and SAWs. Here we present the findings from experiments involving different materials (nickel, cobalt [1], FeSi [2], and FeGa [3]) subjected to high-frequency SAWs ranging from 500 MHz up-to 3 GHz. The experimental set-up, shown on the bottom part of Fig. 1 (a), consists of a piezoelectric and a ferromagnetic thin film. SAWs are generated using Interdigital transducers which in turn interact with the ferromagnetic material, resulting in the generation of MAWs. A representative XMCD image is shown in the top part of Fig. 1 (a), where MAWs are shown on Nickel at two different frequencies. These experimental techniques, together with micromagnetic simulations, allow the quantification of the magnetoelastic constants, which is an indication of the coupling strength between strain and magnetization. Moreover, we have also explored through micromagnetic simulations the effects of SAWs and MAWs on magnetic domain walls (DW), revealing that DW dynamics can be altered depending on the DW characteristics.

[1] M. Rovirola et al. arXiv:2312.15269v1 (2023)

[2] M. Rovirola et al. Phys. Rev. Applied 20, 034052 (2023)

[3] Manuscript in preparation

Broadband ferromagnetic resonance spectroscopy for domain wall resonance measurements

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Abstract

Magnetic domain walls are stable configurations of the magnetization that have been widely studied for spintronic applications in magnetic data storage systems and in data manipulation in a computational way. The oscillatory behavior of the domain walls has attracted attention for its ability to generate microwaves and spin waves, and its potential applications to telecommunications and computing. In order to develop technologies that exploit the oscillatory behavior of the domain walls, a further understanding of the magnetization dynamics must be acquired. In this work we introduce a broadband ferromagnetic resonance spectroscopy technique for the characterization of the magnetization dynamics in ferromagnetic micro and nanostructures. Additionally, we present the ferromagnetic resonance of a domain wall arising in a permalloy microstrip. This domain wall ferromagnetic resonance was measured in the range of 2.0 GHz to 2.8 GHz, and the high slope of the linear dependency of the resonant frequency with the applied magnetic field can be promising for telecommunications and logical computing applications, as before mentioned. The presence of the domain wall in the system could be confirmed by Kerr microscopy and independent

anisotropic magnetoresistance measurements. Finally, we could associate the resonance to the dynamic behavior of the domain wall by an innovative dual transport set-up that allows the simultaneous measurements of broadband ferromagnetic resonance and anisotropic magnetoresistance.

Non-Linear Magnetoresistance due to Magnon Creation-Annihilation in Pt/Y3Fe5O12 Thin Films

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Abstract

Magnons are magnetic excitations in magnetic ordered materials that carry quanta of spin angular momentum. Recent works have shown that non-equilibrium magnons can be electrically excited and detected in magnetic insulators by exploiting charge-to-spin conversion phenomena in heavy metal overlayers [1]. Experiments have mostly focused on investigating magnon injection/detection efficiencies and transport characteristics of the propagating magnons, but the influence of magnon creation and annihilation processes on emerging phenomena in the metal layer has remained overlooked. In our work we demonstrate that the creation and annihilation of magnons driven by an ac current result in emerging non-linear magnetoresistive effects in the metal. In particular, in Pt/Y3Fe5O12(YIG) we found that the changes in the magnetic moment induced in YIG result in a remarkable non-linear planar Hall response in the Pt, which is captured in the second harmonic response. Strikingly, we found a remarkable strong thickness dependence of the effect, even after normalizing the signals by the thickness and Gilbert damping of the YIG layer. We attribute the increase of the signal upon reducing the thickness to the variation of the magnon chemical potential and magnon spectrum density, suggesting a 3D to a 2D-like transition for the magnon band occupation. Moreover, we observe a power law decrease of the amplitude of the magnetic moment induced by the current as the magnetic field increases. This observation correlates with variation of the linear planar Hall response with magnetic field, indicating that effect originates from the modulation of the spin-to-magnon transmission efficiency across the interface Pt/YIG interface. All results point to a dominant contribution of the low frequency (subthermal) magnons to the magnon creation/annihilation effects observed. This phenomenon is expected to be relevant in ultrathin low-damping magnets.

[1] L. Cornelissen et al. Nature Phys. 11, 1022–1026 (2015)

Experimentally studying Bloch point magnetic singularities in thin films and microstructures

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Abstract

The role of topology on magnetic textures is of paramount importance as it has direct impact on their stability, as well as on their behaviour under external stimuli [1,2]. Moreover, the magnetization reversal processes and texture nucleation and propagation through a magnetic material, can be understood in terms of magnetic topological charge conservation rules, which can establish a general framework for the understanding of magnetization transformations [3]. However, in order to perform this characterization, one must first access their three-dimensional magnetization configuration. In this work, we characterize the full vector magnetic configuration of several magnetic systems where Bloch point singularities exist. Specifically, we have analysed Ni₈₀Fe₂₀/NdCo₅/Ni₈₀Fe₂₀ and Gd₁₂Co₈₈/NdCo₅/Gd₂₄Co₇₆ ferromagnetic and ferrimagnetic heterostructures, and Ni₈₀Fe₂₀ microstructures. We use the unique capabilities of Soft X-ray vector tomography to access experimentally their topological characteristics [4] as well as their interactions through the topological emergent field [3]. Finally, we show how is it possible to even engineer the inner magnetic configuration of these textures by tuning the magnetostatic interaction strength at the interface between antiferromagnetically coupled layers [5].

[1] H. Oike et al., Nature Physics 12, 62 – 66 (2016).

[2] K. Litzius et al., Nature Physics 13, 170 – 175 (2017).

[3] J. Hermosa-Muñoz et al., Communications Physics 6, 49 (2023).

[4] A. Hierro-Rodríguez et al., Nature Communications 11, 6382 (2020).

[5] J. Hermosa-Muñoz et al., arXiv:2312.09836 (2023).

Complex two-step magnetisation reversal in bi-modulated cylindrical FeCo nanowires

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Abstract

Control of magnetisation processes in cylindrical magnetic nanowires is very important since these nanostructures can potentially be used as future blocks of three-dimensional magnetic applications [1]. The cylindrical geometry stabilizes a number of novel 3D magnetic textures with increased complexity such as Bloch Point domain walls (DWs) or vortex and skyrmion tubes. Fabrication methods, typically by electrodeposition onto anodised alumina templates, allow for a significant versatility in the engineering of cylindrical structures, including modulations in diameter [2]. In this work, bisegmented FeCo nanowires with a large difference in diameters and a sharp transition have been prepared. We employed variable field magnetic force microscopy (VF-MFM) techniques [3] to investigate the effects of large diameter differences and sharp transitions in the magnetic behaviour of FeCo ferromagnetic nanowires. For the first time, we

clearly observe that the magnetisation process starts in the wider segment as corresponds to the theoretically predicted decrease of coercivity with an increase of diameter. The VF-MFM imaging shows a propagating contrast which starts from the end of the segment of a larger diameter and propagates toward the constriction as the external field increases. The complementary micromagnetic simulations demonstrate a complex two-step magnetisation reversal starting with the injection of Bloch points at the ends of the wider segment, that initiates a propagating vortex/skyrmion tube structure. The narrow segment shows a one-step demagnetization by a transverse domain wall propagation, simultaneous with the core reversal in the wider tube. Thus, the mechanism is consistent with predicted skyrmion-tube structures and the corkscrew pinning mechanism [4,5]. Our results open the possibility for DW devices with the controlled DW injections.

- [1] A. Fernández-Pacheco et al. T. Sci Rep 3, 1492 (2013)
- [2] C. Bran et al., M², Editor: M. Vázquez, Woodhead Publishing, ISBN: 978-0-08-102832-2 (2020)
- [3] M. Jaafar et al., , Nanoscale Research Letters, 6(1), (2011) 6:407.
- [4] E. Berganza et al., Materials (Basel). 14(19):5671 (2021)
- [5] J. Fernandez-Roldan et al., . Nanoscale 2018, 10, 5923–592

Ørsted-field-driven domain wall motion in cylindrical nanowires

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Abstract

Three-dimensional magnetic nanowires could be building blocks for the next generation of spintronic nanodevices, particularly those based on the control of magnetic domain walls (DWs) driven by electric current. Due to a specific topology in such a 3D shape, new curvature-induced effects appear such as the stabilization of curling spin textures or the delay of the Walker breakdown, which allow higher domain wall speeds. It has been recently reported in magnetic nanowires with axial magnetization that local chemical modulations serve as DW pinning sites. However, this system requires high current densities of 10^{12} A/m², which results in stochastic sense of motion. Up to now, there has not been experimental evidence on current-induced domain wall motion in NWs with a diameter above 200 nm, where Ørsted field is expected to lead dynamics over spin transfer torque (STT). We propose a system based on Permalloy cylindrical nanowires of diameter 200 nm with periodic Fe₇₀Ni₃₀ chemical modulations of 40 nm of length. This system presents azimuthal domains due to its large diameter. The nanowires were synthesized using template-assisted electrochemical deposition and electrically contacted using laser lithography on high-resistivity Si substrates with 20 nm thick Si₃N₄ windows. Transmission X-Ray Microscopy (TXM) at ALBA synchrotron was used to access the 3-dimensional magnetization textures. We report deterministic domain-wall motion driven by the circulation of the Ørsted field related to the sign of nanosecond current pulses with an amplitude of the order of 10^{10} A/m², with velocities above 1000 m/s. These current density amplitudes for motion are one order of magnitude lower than previously reported, allowing to attribute the leading dynamics to the Ørsted field. We also evidenced that the length of nucleated domains is proportional to the duration of the applied pulse, indicating that nucleation is not induced by thermal activation.

Magnetic properties dependence of chemical and geometrical modulations in Co-Ni bi-segmented nanowires

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Abstract

In the last decades, the advances in fabrication and characterization techniques have allowed to fabricate metallic and magnetic multisegmented nanowires (NWs) which can exhibit outstanding tailor-made physico-chemical properties. Among them, magnetic anisotropy, coercivity, pinning of magnetic domain walls (DWs) and well-defined magnetization reversal processes, can be precisely controlled by properly tuning the geometrical and compositional modulations of NWs. Even though both modulations have been studied many times on a separate way, both modulations at once have barely been performed due to the difficulties arising from the fabrication processes [1]. In this work, we have fabricated compositionally and diameter modulated Co-Ni bi-segmented NWs, whose composition changes at the interface between the wide and narrow NW segments. Starting nanoporous alumina membranes (NAMs) are made by combining the electrochemical anodization, pore widening and atomic layer deposition (ALD) processes, obtaining a well-defined pores diameter modulation with a sharp transition between the two diameter segments. Afterwards, NAMs are filled by electrodeposition techniques by controlling the current profile, which allows to fill the bi-segmented nanopores with different magnetic materials, thus resulting compositionally and geometrically modulated NWs. Therefore, four different samples were fabricated with a fixed 3:1 ratio in the diameter modulation of bi-segmented NWs and varying the composition of the thinner and wider segments (Co-Co, Ni-Ni and Co-Ni or Ni-Co, respectively). Morphological and compositional analysis were conducted by SEM and HR-TEM techniques. Temperature dependent magnetic hysteresis loops (HLS) have also been performed by VSM to determine the influence of geometrical and chemical modulations on the magnetic behaviour. The intrinsic magnetization reversal of the NW segments and the magnetostatic interactions among NWs, are strongly dependent on all these possible combinations among composition/diameter modulations of the NW segments.

[1] Pitzschel et al. J.Appl.Phys. 109, 033907 (2011)

Large magnetoresistance of isolated domain walls in $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ nanowires

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Abstract

Generation, manipulation, and sensing of magnetic domain walls are cornerstones in the design of efficient spintronic devices. Half-metals are amenable for this purpose as large low field magnetoresistance signals can be expected from spin accumulation at spin textures. Among half metals, $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ (LSMO) manganites are considered as promising candidates for their robust half-metallic ground state, Curie temperature above room temperature ($T_c = 360$ K, for $x = 1/3$), and chemical stability. Yet domain wall magnetoresistance is poorly understood, with large discrepancies in the reported values and conflicting interpretation of experimental data due to the entanglement of various source of magnetoresistance, namely, spin accumulation, anisotropic magnetoresistance, and colossal magnetoresistance. In this work, the domain wall magnetoresistance is measured in LSMO cross-shape nanowires with single-domain walls nucleated across the current path. Magnetoresistance values above 10% are found to be originating at the spin accumulation caused by the mistracking effect of the spin texture of the domain wall by the conduction electrons. Fundamentally, this result shows the importance on non-adiabatic processes at spin textures despite the strong Hund coupling to the localized t_{2g} electrons of the manganite. These large magnetoresistance values are high enough for encoding and reading magnetic bits in future oxide spintronic sensors.

POSTER: Spin-textures dynamics in cylindrical nanowires

Presenter

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Abstract

In the field of spintronics, the study of current-driven magnetization dynamics is crucial for understanding the switching behavior of nano-elements. Three-dimensional nano-objects come with two specific aspects. Firstly, curvature promotes flux-closure of magnetization, resulting in curling textures as an additional degree of freedom. Secondly, the Oersted field may play a significant role in directly influencing the curling structures and determining the timescale of their switching dynamics.

Magnetic cylindrical nanowires provide an optimal platform for exploring 3D nanomagnetism. Curling magnetization, induced by magnetostatics, arises in various forms, such as in the Bloch Point Wall (BPW), azimuthal domains, and in diameter or composition changes. A common feature among all the curling textures is the reversal of its circulation under a nanosecond current pulse of antiparallel Oersted field circulation.

Here, we investigate Permalloy cylindrical nanowires with periodic inserts of Fe-rich chemical modulations, acting either as pinning locations for domain walls, or as sources of intrinsic curling. The nanowires were synthesized using template-assisted electrodeposition and were electrically contacted via laser lithography. Their three-dimensional magnetization was characterized by X-ray magnetic imaging in both static and time-resolved modes. Micromagnetic simulations were employed to track intermediate states of the dynamics.

We focus our investigation on the interplay between the chemical modulations and DWs. The behaviour depends on their relative curling circulation and promotes various types of DW transformations. We also present 50 ps time-resolved experiments for both modulation and BPW switching, allowing for a direct comparison with the micromagnetic simulations. The timescale for the switching of curling at the chemical modulations is 200 ps. In contrast, a significantly longer timescale, typically 1 ns or more, was observed for the switching of BPW circulation. This longer timescale enables deterministic control over the type of DW, whether it be a BPW or Transverse-Vortex wall, or the expulsion of a BPW from a modulation.

POSTER: Asymmetric magnetic response induced by compositional gradients in Ni-Fe nanowires

Presenter

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Abstract

The control over domain wall motion in cylindrical nanostructures is a key factor for developing the next generation of spintronic and logic devices [1,2]. Among several strategies, introducing changes in the chemical structure of the wire (chemical barriers) has been proven to be an effective way to pin the domain walls [3], but determining the direction of domain wall movement still remains as an open challenge. Following the same approach, in this work we introduced gradients of composition in Ni-Fe nanowires to pattern a ratchet profile of domain wall energy along the nanowire axis, in order to create an asymmetry for domain wall movement.

Nanowires were synthesized using template-assisted electrodeposition. The composition was gradually changed between Ni₉₀Fe₁₀ and Ni₃₅Fe₆₅ along the nanowire longitudinal axis in periods of a few micrometers. By combining laterally resolved X-ray Absorption Spectro-microscopy (XAS) and X-ray Magnetic Circular Dichroism (XMCD), we correlated the chemical structure of single nanowires with their 3D spin texture. By applying external magnetic fields along the nanowire axis, we studied the evolution of the magnetic state depending on the field direction. In addition, First Order Reversal Curves (FORC) were also measured in arrays of nanowires with axial gradients and in arrays of nanowires with homogeneous composition (as reference sample). While the diagram of homogeneous nanowires is highly symmetric with respect to the interaction field axis (H_U), an asymmetry arises in the diagram of nanowires with axial gradients, evidencing the emergence of asymmetrical magnetization processes in the nanowires [4].

[1] R. Streubel, et al. J. Phys. D: Appl. Phys. 49 (2016) 363001.

[2] Z. Luo, et al. Nature, 579 (2020) 214.

[3] S. Ruiz-Gómez, et al. Nanoscale, 12 (2020), 16695.

[4] C. Fernández-González, et al. Scrip. Mater. 243 (2024) 115970

POSTER: Generation of intense, polarization-controlled magnetic fields with non-paraxial structured laser beams

Presenter

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Abstract

The ability to spatially separate the electric (E-field) and magnetic (B-field) fields of a light beam enables the inspection of laser-matter interactions driven solely by optical B-fields, covering studies in magnetic spectroscopy, force microscopy, or ultrafast magnetization dynamics among others. As B-field field excitations are commonly orders of magnitude weaker than E-field ones, not only isolated, but also intense B-fields, are required. Several studies have already demonstrated the isolation of an intense, linearly polarized B-field using structured light. However, control over the B-field polarization state is crucial for

certain applications, such as to specifically excite spin textures or to drive nonlinear magnetization dynamics in ferromagnets where circularly polarized B-fields are required. The solution of Maxwell equations of a spatially isolated circularly polarized B-field requires an exceedingly challenging E-field structure, out of the scope with the current laser technology. To circumvent this drawback, we propose the generation of isolated high-intensity magnetic fields using several tightly focused azimuthally polarized laser beams. We report B-fields up to tens of Tesla that can be reached from moderately intense azimuthally polarized laser beams of $\sim 10^{12}$ W/cm². Our theoretical findings, based on the Richards-Wolf vectorial diffraction theory, highlight a significant enhancement in the amplitude of the longitudinal B-field carried by an azimuthally polarized vector beam under tight-focusing conditions. By implementing a multiple-beam configuration, we achieve precise sub-wavelength control over the polarization state of the spatially isolated B-field from a feasible experimental setup point of view, with the possibility to obtain isolated circularly polarized B-fields. The potential applications of the presented work span various scientific and technological scenarios, where precise control over selective E-field and B-field excitations is required. These applications include probing and inducing spin textures, ultrafast dynamics in ferromagnetic materials or chiral media, as well as enhancing spatial resolution in optically controlled magnetization applications.

POSTER: Exploring the Advanced Interaction of Ferrofluids and Magnetic Microwires for Cutting-Edge Biosensor Tecnology

Presenter

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Abstract

The magnetic properties of microwires render them as excellent candidates for biosensor development. Specifically, the phenomenon of magnetoelasticity resonance influenced by a range of physical parameters including microwire length, magnetic field, mass, and other parameters, has demonstrated promising potential for biosensor development [1]. For instance, these sensors have shown a significant ability to interact with a liquid medium, accurately determining the viscosity and density of the liquid [2].

The modulation of magnetic domains dynamics within the microwire, influenced by their interactions with magnetic nanoparticles, supports the notion that combining ferrofluids and microwires can result in promising biosensors based on magnetoelastic resonance. This coupling between magnetic nanostructures and the microwire domains can alter the magnetoelastic resonance, a phenomenon that can be harnessed to enhance sensors that rely on this property.

Magnetoelastic resonance in a microwire composed of an Fe-Nb alloy has been assessed under various conditions: in air, in distilled water, with dry magnetite magnetic nanoparticles on its surface, and in a ferrofluid state at differing concentrations. In all the scenarios mentioned, a distinct variation in the magnetoelastic resonance was observed. It has been demonstrated that external modifications to the

nanoparticles influence the resonance and, consequently, the dynamics of the domains. Preliminary data suggest that this principle can be utilized across a wide range of biosensors.

Thus, while the magnetic properties of microwires and nanoparticles each hold promise for biosensor development, their synergetic combination could lead to the creation of advanced wireless biosensors that are reusable, provide real-time measurements, are cost-effective, and eco-friendly.

[1] A. Peña, et al.(2022). *Biosensors*. DOI:10.3390/bios12100871.

[2] P. Marín, et al.(2010). *Appl Phys Lett*. 96. <https://doi.org/10.1063/1.3459140>.

POSTER: Mechanisms of current driven Néel vector reorientation in Mn₂Au

Presenter

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Abstract

Current pulse driven Néel vector reorientation in metallic antiferromagnets (AFM) is one of the most promising concepts in antiferromagnetic spintronics. We have shown that such reorientation can be achieved in the metallic antiferromagnet Mn₂Au through two distinct mechanisms [Rei2023]. The first mechanism is the bulk Néel spin orbit torque, which originates from the unusual crystal structure of Mn₂Au in conjunction with strong spin-orbit coupling. The second mechanism originates from magnetoelastic coupling associated with current driven heating effects. In order to separate these two mechanisms experimentally, we use different geometries to alter the current path, thus changing the strain pattern. Additionally, we modify the pulse duration to reduce the heating. We show that both effects are present with the thermomagnetoelastic being dominant for longer pulse lengths. We use XMLD-PEEM with in-situ current pulsing together with AMR measurements to probe the reorientation of the Néel vector. [Rei2023] Reimers, S., et al. Current-driven writing process in antiferromagnetic Mn₂Au for memory applications. Nat. Commun.14, 1861 (2023).

POSTER: Perpendicular Magnetic Anisotropy and Magneto-Optical Signal of [Co/Pt]₁ Ultra-Thin Films

Presenter

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Abstract

Magnetic ultra-thin films with perpendicular magnetic anisotropy (PMA) are interesting metamaterials due to their potential for technological applications, particularly in the fields of magneto-optical recording, high-density magnetic storage and spintronics. Magnetron sputtering is the usual technique for fabricating continuous thin films of this kind, offering high quality multilayers and good control on critical growing parameters. However, its deposition geometry makes difficult to integrate with nanopatterning, often giving rise to problems with the quality of the edges of the nanostructures. In this work, we demonstrate an approach for growing electron beam evaporated ultra-thin films made of a single Co/Pt repetition (below 1 nm) with high degree of PMA with the help of a Cu buffer layer. Electron beam evaporation (EBE) is a non-conformal and accessible physical vapor deposition technique compatible with nanolithography, providing an easy path to study the magnetic properties of patterned materials. High quality PMA was obtained at a relative high deposition pressure instead of conventional ultra-high vacuum conditions. The addition of a Cu underlayer plays a key role to promote sharp PMA at these conditions by enhancing the (111) growth of Pt and increasing interfacial roughness. The control of the Cu and Pt underlayer thicknesses makes possible to fine-tune the coercive field while maintaining a well-defined squareness in the out-of-plane hysteresis loops. The influence of the Cu layer on the magneto-optical Kerr signal was also studied, showing a correlation between the increase in coercivity and the weakening of the Kerr amplitude as the buffer layer grows. Work supported by PID2022-136784NB-C22 funded by MCIN/AEI/ 10.13039/501100011033, by “ERDF A way of making Europe” by the “European Union”, and by Department of Education of the Basque Government through the PIBA project call (PIBA_2021_1_0051).

POSTER: Current induced propagation of magnetic vortices in NdCo5/Ni8Fe2 bilayers: memory effects and SOT

Presenter

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Abstract

Over the last decade an extensive field of study surrounding the magnetic racetrack paradigm has been developed, and it is focused on achieving low energy consumption energy devices. Here we analyze the performance of a reconfigurable racetrack that can be designed as a multilayer of NdCo5/ Ni8Fe2. The hard magnetic material with weak Perpendicular Magnetic Anisotropy (NdCo5) presents a stripe domain configuration that can be imprinted in the soft magnetic material (Ni8Fe2). This pattern hosts spin textures with well defined topological charges and establishes paths for the propagation [2]. We have studied the propagation of spin textures along the stripe domain pattern under the effect of pulsed currents and considering magnetic history and externally applied fields. MTXM experiments show guided

vortex/antivortex (V/AV) propagation events within the Ni₈Fe₂ over a threshold current of 10^{11} A/m². Opposite propagation senses have been observed depending on the topological charge of the spin texture, both in the remanent state and when there is an external field being applied. The propagation sense does not depend on the sign of the applied current and there is no topological hall effect, implying that this is a thermally activated phenomenon. Micromagnetic simulations of our multilayer reveal that the guiding effect and the asymmetries in propagation sense are due to the magnetic history of the NdCo₅. There is an exchange-bias effect that controls the propagation of the textures depending on the last in plane saturation sense of the hard layer. This exchange energy acts as a magnetic spring selecting a favourable sense for the movement of the V/AV pairs. The equivalent bias field related to this exchange spring has been estimated to be $|\mu_0 \cdot H_{\text{bias}}| \approx 10$ mT. The SOT effects induced adding a top Pt layer have also been studied.

[2] A. Hierro-Rodriguez et al., APL, 110, 26 (2017).

POSTER: Current-driven orbital angular momentum flow from Cu/oxide interfaces

Presenter

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Abstract

The angular momentum of the electrons can be used to manipulate the magnetic moments in thin films [1]. Most applications, however, involve spin-orbit coupling (SOC) which is limited to a few number of materials. Orbital angular momentum (OAM) in light materials has appeared as an interesting alternative to the use of spin, yet holding better efficiencies [2]. Deploying OAM currents in experiments might be challenging, because conversion of orbital into spin currents is necessary for transferring angular momentum to the spin-lattice. This conversion is achievable by interfacing the OAM generator with a SOC metal [3], highlighting a critical step in the experimental validation and utilization of OAM in device applications.

In our study, we explore the generation and propagation of OAM at copper (Cu)/oxide interfaces [4]. The OAM generation is assessed via spin-orbit torque (SOT) measurements in Co/Pt bilayers interfaced with our OAM generator. Such analysis is performed at room temperature via harmonic magneto-transport measurements in patterned hall-bar devices [5]. In our study, we find that orbital currents significantly enhance SOT in Co, as evidenced by an enhanced damping-like (DL) torque in the second harmonic response. By interfacing copper (Cu) with AlO_x and CuO_x, we demonstrated a threefold enhancement of the DL torque in Co compared to the reference Co/Pt bilayer. Therefore, the use of OAM currents results in a massive enhancement of the angular momentum transfer to the magnetic lattice. These results highlight the potential of *orbitronics* to extend the range of materials to be employed in the next generation of electronic devices.

[1] A. Hirohata et al., *JMMM* 509, 166711 (2020).

[2] D. Go et al., *EPL* 135, 3 (2021).

[3] S. Ding et al., *PRL* 125, 177201 (2020).

[4] J. Kim et al., *PRMat* 7, L111401 (2023).

[5] S. Ding et al., *PRL* 128, 67201 (2022).

POSTER: Growth and Characterization of Ir_{1-x}Co_xO₂ Thin Films

Presenter

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Abstract

IrO₂ is one of the most promising materials for spin-current detection applications due to the high spin-orbit coupling (SOC) of the Ir ions that makes possible an efficient conversion of pure spin-currents on charge-currents via the so-called inverse spin Hall effect (ISHE) [1, 2]. In order to improve the performance of IrO₂ as spin detector doping with different elements appears as a natural route. Indeed, in the current quest for optimized spintronic materials, doping is one of the most feasible and commonly used methods to modify the electronic structure of the host compounds [3,4]. The different ionic size of the dopant may give rise to contraction/elongation of the lattice and/or distortions that can significantly change the electronic structure. Similarly, the dopant ions can induce relevant changes in the oxidation state of the host. In addition, when a magnetic ion is inserted in the lattice it can give rise to the appearance of magnetic ordering and Slater- insulator behaviors. The doping of IrO₂ with 4+ ions, such as Sn⁴⁺ and Cr⁴⁺, has been reported to give rise to strong changes in its electronic and/or magnetic behavior [5,6]. On the other hand, the effect of increasing the oxidation state of Ir in IrO₂ films has remained unexplored to date, even when in other iridium oxide series a larger SOC has been reported for Ir⁵⁺ relative to Ir⁴⁺ [7]. Here, Ir_{1-x}Co_xO₂ thin films have been prepared by reactive magnetron co-sputtering deposition. Composition, structure, oxidation state and magnetic behavior have been analyzed. After annealing, an Ir_{1-x}Co_xO₂ substitutional solid solution phase was achieved for a wide Co-doping range (0 ≤ x ≤ 0.6). In all the cases a rutile crystal structure was found even when no binary Co oxide crystallizes in this structure. XAS spectra show that the oxidation state of cobalt is Co³⁺ and that this triggers an increase in the oxidation state of Ir, up to ~ 5+ in the Ir_{0.6}Co_{0.4}O₂ sample. By application of sum rules, a 13% increase in the SOC is found despite the fact that lattice shrinkage causes a detrimental bandwidth broadening. In addition, our work shows that the magnetic response of the doped films is very similar to that of the paramagnetic parent IrO₂. No enhancement of the susceptibility is observed indicating a non-magnetic low spin Co³⁺ electronic configuration. This results indicate a route for further optimization of the performance of the IrO₂ as spin current detectors.

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- [1] K. Fujiwara et al., Nat. Commun. 4 (2013) 2893
- [2] M. Morota et al., Phys. Rev. B 83 (2011) 174405
- [3] N. Che Ani et al., Materials Science and Engineering: B 276 (2022) 115536
- [4] V. K. Dwivedi and S. Mukhopadhyay, Journal of Applied Physics 126 (2019) 165112
- [5] E. Arias-Egido, et al., Adv. Funct. Mater. 29 (2019) 1806754
- [6] E. Arias-Egido et al., , Materials & Design, 196 (2020) 109083
- [7] M. A. Laguna-Marco et al., Phys. Rev. B 91 (2015) 214433

POSTER: Dielectrophoresis as a tool for the study of magnetic and transport properties in single FeCo and Py nanowires

Presenter

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Abstract

Dielectrophoresis (DEP) refers to the force exerted on the induced dipole moment of an uncharged particle by a nonuniform electric field [1]. Since then, it has been widely used as a technique for the manipulation of microscale and nanoscale objects in areas ranging from industrial processing to small scale biotechnology [2].

In our work, we have employed dielectrophoresis to align metallic nanowires [3] and place them in appropriate locations to facilitate the study of their magnetic and transport properties. With this goal, we have designed devices in which one or various nanowires can be easily positioned by means of the dielectrophoretic force generated. This is achieved by applying a high frequency AC electric field between a pair of electrodes separated by a gap of a few microns. We have also developed a MatLab code that allows to catch a single nanowire. As a proof of concept, we demonstrate the utility of this code with carbon nanotubes and evaluate the difficulties that arise when working with magnetic (FeCo and permalloy) nanowires. This setup would be a key factor in the study of individual nanowires, one of the most promising research areas in 3D nanomagnetism.

[1] Jones, T. B. Dielectrophoresis and magnetophoresis. In: *Electromechanics of Particles*. Cambridge University Press; 1995:34-82.

[2] Sarno, B., Heineck, D., Heller, M.J. and Ibsen, S.D. (2021), Dielectrophoresis: Developments and applications from 2010 to 2020. *ELECTROPHORESIS*, 42: 539-564.

[3] Puydinger dos Santos, M. V., Lima, L. P. B., Mayer, R. A., Béron, F., Pirota, K. R., Diniz, J. A.; Dielectrophoretic manipulation of individual nickel nanowires for electrical transport measurements. *J. Vac. Sci. Technol. B* 1 May 2015; 33 (3): 031804.

POSTER: Morphology and dynamics of domain walls through asymmetric hole 2D-arrays

Presenter

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Co-presenter

María Ángeles Laguna Marco INMA (CSIC-Universidad de Zaragoza)

Abstract

The manipulation of magnetic domain walls (DW) opens novel strategies to design spintronic devices with potential high impact in data storage, nonvolatile logic, and magnonic applications, which may include reservoir/neuromorphic computing, data storage, and sensors among others. For the implementation of several of those applications, asymmetric DW motion controlled by electrical voltages or currents and magnetic fields is needed. The prototypical asymmetric DW motion mechanism is the so-called ratchet effect, which consists of an easier propagation of domain walls in one direction than in the other thanks to an asymmetric pinning potential.

Different mechanisms have been demonstrated to favour ratchet effect, being patterning into an asymmetric configuration one of the preferred options. 2D micropatterned arrays of asymmetric holes (2D-AAH) on magnetic thin films have been reported to show ratchet effect. In the large size regime ($> 10 \mu\text{m}$), the DWs can be approximated as elastic lines of zero width that can distort (i.e. bend) throughout their length when pushed by a magnetic field; being this bending the main factor determining DW propagation. However, in 2D-AAH, the optimum hole size for the occurrence of ratchet effects is twice the DW width. Therefore, when matching the hole size to the DW width of the particular magnetic thin film used, the DWs cannot be considered 1D objects but their morphologies play a very important role. Indeed, not only the bending of the DW determines the depinning processes, but also the edge half vortex with $\pm 1/2$ topological charge at the top and bottom of the asymmetric holes. To disentangle the main structural parameters affecting the DW dynamics, we have combined Kerr microscopy and X-Ray PhotoEmission Electron Microscopy to study 2D-AAHs with different hole shapes, sizes, and pattern structure, and we have determined how these features affect the dynamics of the DW.

Light-matter interactions in 2D materials (DFMC-GEFES) / Interacción luz-materia en materiales 2D (DFMC-GEFES)

Organiser

Reyes Calvo (U Alicante) Alexey Nikitin (DIPC) Pablo Alonso-González (U Oviedo) Blanca Biel (U Granada)

Invited speakers

Rainer Hillenbrand (CIC nanoGUNE) Miguel Anaya (ICMS, U. Sevilla-CSIC) Marta Galbiati (U. Valencia) Julen Ibañez (CFM-CSIC) Georgia Papadakis (ICFO) Karolina Slowik (U. Nicolaus Copernicus) Luis Martín-Moreno (INMA, CSIC) Saul Velez (UAM, IFIMAC) Aitana Tarazaga (U. Oviedo) María Asensio (ICMM)

Symposium abstract

In the last decade, research activity on light-matter interactions in atomically thin (2D) materials has grown dramatically. Two-dimensional materials provide a unique platform for the study of new physical phenomena that emerge from their inherent low dimensionality, as well as those that can be obtained through the stacking of these materials in hetero- and homostructures. Our symposium "Light-matter interactions in 2D materials" will cover novel optical and optoelectronic phenomena in 2D materials and will provide a framework where researchers from various fields can meet. It will cover classical and quantum optics; many-body phenomena in light-matter interaction; non-linear optical response, near-field microscopy, topological photonics; among many others. The symposium will thus provide a framework in which unifying concepts can be formed, new ideas inspired and new frontiers in theoretical and experimental research in light-matter interaction in 2D materials.

En la última década, la investigación en las interacciones entre la luz y la materia en materiales bidimensionales (2D) ha crecido de manera significativa. Los materiales bidimensionales ofrecen una plataforma única para el estudio de nuevos fenómenos físicos que surgen de su inherente baja dimensionalidad, así como de aquellos que pueden obtenerse mediante el apilamiento de estos materiales en hetero- y homoestructuras. Nuestro simposio "Interacciones luz-materia en materiales 2D" abordará fenómenos ópticos y optoelectrónicos novedosos en materiales 2D y proporcionará un marco donde los investigadores de diversos campos puedan encontrarse. El simposio cubrirá distintos aspectos de óptica clásica y cuántica; fenómenos many-body en interacción luz-materia; respuestas ópticas no lineales, espectroscopías de campo cercano; fotónica topológica, entre muchos otros. El simposio proporcionará, por lo tanto, un marco en el cual se pueden formar conceptos unificadores, inspirar nuevas ideas y abrir nuevas fronteras en la investigación teórica y experimental de la interacción luz materia en los materiales 2D.

List of abstracts at the symposium

Electronic nano-imaging and Nano-ARPES: An innovative and powerful tool for the nanoscience

1st author

María Asensio ICMM, CSIC

Abstract

We have witnessed exponential advances in new nanotechnologies based on low-dimensional materials in recent decades. These nanomaterials had shown remarkable properties; however, they would have remained unexploited if, at the same time, we had not developed new tools capable of viewing and scrutinizing objects on a wide range of scales, from a few microns to a few tens of nanometers. Recently, significant progress has been made due to the rapid expansion in the range of modern microscopies, which have successfully achieved nanometer spatial resolution. Nevertheless, the challenge remains to provide

powerful high-energy-resolution spectroscopic tools at the nanoscale. To accomplish this goal, the electronic structure must be measured not only regarding the detection of core levels. The electronic structure of delocalized valence bands must also be recorded because these electronic states are directly responsible for chemical bonds, electrical transport, and thermal and mechanical properties.

Traditionally, angle-resolved photoemission spectroscopy (ARPES) is the only technique capable of making sufficiently precise measurements of the dispersion of the band structure of materials in the reciprocal space. We have developed an electronic nano-scope based on the ARPES principles, which can perform spatially resolved ARPES experiments on the nanometer scale. In this presentation, we will review several results of our group using the Nano-ARPES1 technique. This sophisticated instrument can have a high spatial resolution in several tens of nanometers of real space. That allows the direct imaging of core levels and their chemical shifts, band electronic structures in reciprocal space. Low-dimensional materials of a few atomic layers have been investigated in silicene, graphene multilayers with different stacking, Moiré structures, topological surfaces, and many others.²

[1] Nano-ARPES, Wikipedia. Website: <https://en.wikipedia.org/wiki/Nano-ARPES>

[2] Z. Gao, et al., Large-area epitaxial growth of curvature-stabilized ABC trilayer graphene, Nat Commun 11 (2020) 546. <https://doi.org/10.1038/s41467-019-14022-3>.

Managing light-matter interactions in halide perovskites for enhanced optoelectronic devices

1st author

Miguel Anaya ICMS, U Sevilla- CSIC

Far-field thermal photonics with polaritonic materials

1st author

Georgia T. Papadakis ICFO-Barcelona

Abstract

The blackbody spectrum peaks within the mid-infrared (IR) spectral range for near-room temperatures. In the mid-IR range, most dielectric materials exhibit pronounced phonon polariton resonances. In this talk, I will discuss means of harnessing such resonances to control the bandwidth, directionality, and state of polarization of thermal emission and radiation. First, I will demonstrate that single flakes of low-dimensional materials such as α -MoO₃ or V₂O₅ suffice to achieve mid-IR phase retardation, based on which we have built the thinnest reported phase retarders to date [1]. Harnessing the extreme anisotropy of such flakes can also yield pronounced chiral response in the mid-IR range, which we probe in thermal emission experiments. By leveraging the ultra-low-loss of phonon polaritons supported in low-dimensional materials, for instance in hexagonal boron nitride, I will demonstrate the possibility to induce antenna-like thermal emission lobes with extreme directionality, comparable to that of grating structures [2], but realizable without any lithography [3]. I will demonstrate experimental results of such pattern-free directional thermal emission from polar materials.

A practical challenge arises in the characterization of low-dimensional exfoliated flakes at mid-IR frequencies: retrieving their dielectric properties is unattainable with standard methods like spectroscopic ellipsometry, due to the mismatch between the large size of a mid-IR beam and the small (hundreds of micrometers) size of exfoliated flakes. Previously, near-field methods have been employed for the extraction of the dielectric properties, nonetheless these are subject to considerable numerical fitting. I will introduce an approach to directly obtain the dielectric function of micro-sized-flakes using standard Fourier Transform IR Spectroscopy (FTIR) [4]. Finally, I will present the mid-IR dielectric response of another class of low-dimensional materials, transition metal dichalcogenides. Although their properties at visible frequencies are well-understood, the aforementioned practical challenge has delayed their mid-IR

characterization. I will demonstrate that transition metal dichalcogenides have pronounced phonon resonances at IR frequencies that are suitable for applications in thermal photonics.

- [1] M. T. Enders, M. Sarkar, M. Giteau, A. Deeva, H. Sheinfux, M. Saremi, F. Koppens, G. T. Papadakis, *Nature Communications Materials* 5, 16 (2024), Deeply subwavelength mid-IR infrared phase retardation with a-MoO₃ flakes
- [2] J.-J. Greffet, R. Carminati, K. Joulain, J.-P. Mulet, S. Mainguy, and Y. Chen, *Nature*, 416 (6876) (2002), Coherent emission of light by thermal sources
- [3] M. Sarkar, M. M. Enders, G. T. Papadakis, *Nanophotonics* 0595 (2023), Lithography-free directional control of thermal emission
- [4] M. Sarkar, M. M. Enders, M. Shokooh-Saremi, K. Watanabe, T. Taniguchi, H. Sheinfux, F. Koppens, G. T. Papadakis, arxiv:2305.13994 (2023), Retrieving optical parameters of emerging van der Waals flakes,

IR and THz nanoscopy of ultra-confined phonon and plasmon polaritons

1st author

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Abstract

Phonon and plasmon polaritons – light strongly coupled to optical lattice vibrations and electron oscillations, respectively - can exhibit ultra-short wavelengths, long lifetimes and strong field confinement, which allows for manipulating IR and THz fields at the nanometer scale. Here we use scattering-type scanning near-field optical microscopy (s-SNOM) and nanoscale Fourier transform (nano-FTIR) spectroscopy to study in real space strong light-matter interaction between IR phonon polaritons in h-BN nanoresonators and molecular vibrations in adjacent organic layers, IR phonon polaritons in large-scale CVD grown h-BN multilayers and in-plane anisotropic THz plasmon polaritons in monoclinic silver telluride platelets.

Nanofabrication for light control in two dimensional materials

1st author

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Abstract

Polaritonic excitations in two-dimensional materials have great potential for the development of nanophotonic and optoelectronic applications including mid-infrared to terahertz photodetectors, optical modulators, thermal management, biosensing, and light canalization in flatland optics [1]. The development of efficient devices critically depends on the precise control of the polaritonic excitations and their confinement at the nanoscale.

In this talk we will show how we can produce high-quality nanostructures from flakes of two different type of two-dimensional materials, namely graphene and h-BN, by employing high-resolution electron beam lithography, high vacuum metal deposition, and combined chemical and physical etching processes. We will further explore the plasmonic properties of the nanostructures at the infrared spectra via near-field optical nanoscopy and show that plasmons in graphene and phonon polaritons in h-BN can be used to produce high-quality nanoresonators [2], linear antennas [3], waveguides presenting both volume and surface modes [4], metasurfaces exhibiting hyperbolic dispersion for light canalization [5], polaritonic crystals [6], and molecular sensors operating at the strong-coupling limit [7].

- [1] T. Low et al., *Nat. Mater.* 16, 182 (2017); D.N. Basov, M.M. Fogler & F.J. García de Abajo, *Science* 354, 195 (2016).
- [2] A.Y. Nikitin et al., *Nature Photon.* 10, 239 (2015).

- [3] F.J. Alfaro-Mozaz et al., Nat. Comm. 8, 15624 (2018).
- [4] I. Dolado et al., Adv. Mat. 32, 1906530 (2020).
- [5] P. Li et al., Science 359, 892 (2018) and Nat. Comm. 11, 3663 (2020)
- [6] F.J. Alfaro-Mozaz et. al., Nat. Comm. 10, 42 (2019) & Nano Lett. 21, 7109 (2021).
- [7] M. Autore et al., Light:Science & Appl. 7, 17172 (2018); Dolado et. al., Nat. Comm 13, 6850 (2022).

Fundamentals of polaritons in strongly anisotropic thin crystal layers

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Abstract

Polaritons in strongly anisotropic thin layers have recently captured considerable attention in nanophotonics because of their directional propagation at the nanoscale, which offers unique possibilities for nanooptical applications. However, exploiting the full potential of anisotropic polaritons requires a thorough understanding of their properties, including field confinement, energy and phase propagation direction and losses. Here we provide novel insights on some fundamental aspects of the propagation of anisotropic polaritons in thin biaxial layers. In particular, we introduce a novel methodology that allows us to represent isofrequency curves of polaritons in strongly anisotropic materials considering that the real and imaginary parts of the wavevector are not parallel. In fact, we analytically show that the direction of the imaginary part of the wavevector is parallel to the group velocity and Poynting vector, which can have different, even perpendicular or opposite, directions with respect to the phase velocity. This finding is crucial for understanding polaritonic phenomena in anisotropic media, yet it has so far been widely overlooked in the literature. Additionally, we introduce a criterion for classifying the polaritonic modes in biaxial layers into volume and surface categories and analyze their dispersion, field structure, and losses. Finally, we discover the existence of previously unexplored anisotropic transverse-electric-like modes, which can exhibit natural canalization. Taken together, our results shed light on hitherto unexplored areas of the theory of electromagnetic modes in thin biaxial layers. Although exemplified for van der Waals MoO_3 layers, our findings are general for polaritons in other strongly anisotropic biaxial hyperbolic crystals.

Large Biaxial Compressive Strain Tuning of Neutral and Charged Excitons in Single-Layer Transition Metal Dichalcogenides

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Abstract

The absorption and emission of light in single-layer transition metal dichalcogenides are governed by the formation of excitonic quasiparticles. Strain provides a powerful technique to tune the optoelectronic properties of two-dimensional materials and thus to adjust their exciton energies. The effects of large compressive strain in the optical spectrum of two-dimensional (2D) semiconductors remain rather unexplored compared to those of tensile strain, mainly due to experimental constraints. Here, we induced large, uniform, biaxial compressive strain ($\sim 1.2\%$) by cooling, down to 10 K, single-layer WS₂, MoS₂, WSe₂, and MoSe₂ deposited on polycarbonate substrates. We observed a significant strain-induced modulation of neutral exciton energies, with blue shifts up to 160 meV, larger than in any previous experiments. Our results indicate a remarkably efficient transfer of compressive strain, demonstrated by gauge factor values exceeding previous results and approaching theoretical expectations. At low temperatures, we investigated the effect of compressive strain on the resonances associated with the formation of charged excitons. In WS₂, a notable reduction of gauge factors for charged compared to neutral excitons suggests an increase in their binding energy, which likely results from the effects of strain added to the influence of the polymeric substrate.

Strong light-matter coupling in ultra small-volumes

1st author

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Abstract

This presentation explores several instances of strong coupling between light and vibrations in materials confined to very small volumes. By investigating a variety of configurations, including atomically thin materials and conductors, I will demonstrate that these interactions can be effectively described using the framework of strong coupling.

Monolayer-to-Mesoscale Modulation of the Optical Properties in 2D CrI₃ Mapped by Hyperspectral Microscopy

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Abstract

The recent development of 2D materials with intrinsic magnetism has sparked tremendous interest in the study of 2D magnetism and in the development of magneto-optic devices [1]. However, to achieve the full potential of magnetic 2D materials we require a deep fundamental understanding of their optical properties, still missing today [2]. In this work we implement hyperspectral wide-field transmission imaging as a high throughput non-invasive technique to acquire in a single shot the light intensity coming from tens of CrI₃ crystals with different thickness [3]. To extract the complex dielectric function, we model the spectral information using a Drude-Lorentz model as a function of the layer number, relying on large statistics and simultaneous fit of multiple spectra to increase the consistency of our analysis. Remarkably, we reveal a non-monotonic thickness dependence of the complex optical dielectric function across different length scales. The crossover of the optical properties from bulk to an intermediate multilayer regime at mesoscale hints at a remarkable modification of the electronic properties of the material, which could finally underpin the long-standing magneto-structural conundrum of CrI₃ and provide a fine knob to control the optical properties of the material. This first evidence of the modulation of the intrinsic optical properties of a van der Waals material with an unprecedented evolution starting in the single layer and stretching up to more than 100 layers will have deep implications on the understanding of the scaling of the physical properties with crystal thickness and provides one of the most ample tunable ranges known in van der Waals materials, pushing the boundaries of the modulation of properties of 2D materials with layer number.

[1] Huang et al., Nature 546, 270–273 (2017).

[2] Li et al., Nano Lett. 21, 7602-7608 (2021).

[3] Galbiati et al., PRL (2023).

Bulk photovoltaic effect in 2D-like structures

1st author

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Abstract

The bulk photovoltaic effect (BPE) is the nonlinear optical effect that relates the generation of a dc photocurrent to light absorption in a homogeneous material. It finds its origin in the imbalance of carrier motion along different directions of the Brillouin zone and gives rise to particularly large measured photovoltages [1]. While traditionally the BPE has been predominantly studied in bulk ferroelectrics, the progress in materials synthesis undergone in the past years has allowed measuring it in 2D-like structures such as layered Weyl semimetals [2,3,4] and transition metal dichalcogenide nanotubes [5,6].

In this talk, we will first review the basics of the BPE by discussing the microscopic origin of the process [7] and describe a way of evaluating it in the electronic structure framework based on Wannier functions [8]. We will then discuss its properties by combining the predictions of theoretical calculations and recent optical measurements. Among other effects, we will study the role of topology and Weyl points as well as the importance of excitons and many-body effects in the nonlinear current generation in 2D.

[1] von Baltz and Kraut, Phys. Rev. B 23, 5590 (1981)

[2] Ma, et al., Nat. Mater. 18, 476 (2019).

[3] Puente-Uribe, Tsirkin, Souza and Ibañez-Azpiroz, Phys. Rev. B 107, 205204 (2023)

[4] Sivianes and Ibañez-Azpiroz, Phys. Rev. B 108, 155419 (2023)

[5] Zhang, et al., Nature, 570, 7761, 349 (2019)

[6] Krishna, Garcia-Goiricelaya, de Juan, and Ibañez-Azpiroz, Phys. Rev. B 108, 165418 (2023)

[7] Sipe and Shkrebti, Phys. Rev. B 61, 5337 (2000)

[8] Ibañez-Azpiroz, Tsirkin and Souza, Phys. Rev. B 97, 245143 (2018)

Multiple and spectrally robust photonic magic angles in reconfigurable alpha-MoO₃ trilayers

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Abstract

The recent assembly of van der Waals (vdW) material stacks has unveiled numerous physical phenomena, as it provides a means to accurately control and harness electronic band structures. This has given birth to the so-called field of twistronics. An analogous concept has been developed for highly confined polaritons [1][2], or nanolight, in twisted bilayers of strongly anisotropic vdW materials [3], extending the field to the twistoptics. In this case, the emergence of a topological transition of the polaritonic dispersion at a given twist angle (photonic magic angle) results in the propagation of nanolight along one specific direction (canalization regime), holding promises for unprecedented control of the flow of energy at the nanoscale. However, there is a fundamental limitation in twistoptics that critically impedes such control: there is only one photonic magic angle (and thus canalization direction) in a twisted bilayer, and it is fixed for each incident frequency. Here, we overcome this limitation by demonstrating the existence of multiple spectrally robust photonic magic angles in reconfigurable twisted vdW trilayers.

As a result, we show that the canalization of polaritons can be programmed at will along any desired in-plane direction in a single device with broad spectral ranges. These findings open the door for nanophotonics applications where on-demand control is crucial, such as thermal management, nanoimaging, or entanglement of quantum emitters.

[1] Low, T. et al., Nat. Mater. 16, 182 (2016).

[2] Ma, W., Alonso-González, P., Li, S. et al., Nature 562, 557–562 (2018); Chen, M., Lin, X., Dinh, T.H. et al., Nat. Mater. 19, 1307–1311 (2020) // Z. B. Zheng et al., Nano Lett., 20, 7, 5301–5308, (2020) // Guangwei Hu, et al., Nature 582(7811):209-213, (2020) // Duan, J. et al., Nano Lett. 20, 5323–5329 (2020).

[3] 1. Duan, J. et al., Nano Lett. 20, 5323–5329 (2020).

Optoelectronic interactions of quantum emitters with low-dimensional nanoantennas

1st author

Karolina Slowik U. Nicolaus Copernicus

Abstract

We explore the electronic excitation dynamics in quantum emitters optically and electronically coupled to low-dimensional nanoantennas, taking into account their atomistic arrangements. For this purpose, we develop an efficient tight-binding-based time-domain framework, within which one can coherently capture optical and chemical interactions. The framework is applied to study graphene quantum dots or polyene and polyacetylene molecules via the Su-Schrieffer-Heeger model. We find two distinct interaction regimes depending on the electron tunnelling rate, from the Purcell limit to full hybridisation, as determined by the distance between the nanoantenna and the emitter. Finally, we characterise the optical resonances of the nanoantennas through the proposed energy-based plasmonicity index (EPI). The EPI measures the collective contribution to the resonance in the energy space. This provides a new perspective on plasmons at the atomistic scale, complementary to existing approaches focused on real-space characteristics, beyond the limitations of classical plasmonics in describing these phenomena.

Origin of discrete donor–acceptor pair transitions in 2D Ruddlesden–Popper perovskites

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Abstract

Two-dimensional (2D) van der Waals nanomaterials have attracted considerable attention for potential use in photonic and light-matter applications at the nanoscale. Thanks to their excitonic properties, 2D perovskites are also promising active materials to be included in devices working at room temperature. In this work, we study the presence of very narrow and spatially localised optical transitions in 2D Lead Halide Perovskites by micro-photoluminescence and time-decay measurements. These discrete optical transitions are characterized by sub meV linewidths (~ 120 meV) and long decay times (5-8 ns). X-Ray Photoemission and DFT calculations have been employed to investigate the chemical origin of electronic states responsible of these transitions. The association of Phenethylammonium with Methylammonium cations into 2D Ruddlesden-Popper perovskites, $(\text{PEA})_2(\text{MA})_n\text{Pb}_{n+1}\text{I}_{3n+1}$, particularly in phases with $n \geq 2$, has been identified as a mechanism of donor-acceptor pair (DAP) formation, corresponding to the displacement of lead atoms and their replacement by methylammonium. Ionized DAP recombination is identified as the most likely physical source of the observed discrete optical emission lines. The analysis of the experimental data with a simple model which evaluates the coulombic interaction between ionized acceptors and donors returns a donor bohr radius of the order of ~ 10 nm. This study opens new routes for optimization and development of future outstanding quantum and optoelectronic devices based on 2D Lead Halide Perovskites by means of DAP compositional engineering.

Revealing the existence of out-of-plane trion emission in monolayer WSe₂

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Abstract

Manipulation of light emitted by two-dimensional semiconductors grounds forthcoming technologies in the field of on-chip communications [1-3]. However, these technologies require from the so elusive out-of-plane photon so The urces to achieve an efficient coupling of radiated light into planar devices [4-10]. Here we propose a versatile spectroscopic method that enables the identification of the out-of-plane component of dipoles. The method is based on the selective coupling of light emitted by in-plane and out-of-plane dipoles to the whispering gallery modes of spherical dielectric microresonators, in close contact to them. We have applied this method to demonstrate the existence of dipoles with an out-of-plane orientation in monolayer WSe₂ at room temperature [11]. Micro-photoluminescent measurements, numerical simulations based on finite element methods, and ab-initio calculations have identified trions as the source responsible for this out-of-plane emission, opening new routes for realizing on-chip integrated systems with applications in information processing and quantum communications. For instance, results reported here would allow to identify, at any temperature, potential sources for radially polarized light in monolayer transition-metal dichalcogenides, which may have applications in imaging, phase modulation, and diffractive optics, due to the cylindrical symmetry of their light. Also, this method opens up new routes for the realization of planar devices efficiently exploiting the fundamental properties of atomically thin materials. Finally, it should be mentioned that the proposed technique does not require magnetic fields and can be easily implemented, making it accessible, versatile, and technologically relevant.

[1] R. Won, et al. Nat. Photonics 4, 882 (2010).

[2] S. H. Bae, et al., Nat. Mater. 18, 550–560 (2019).

[3] Z. Jia, et al., ACS Appl. Mater. Interfaces 11, 20566–20573 (2019).

[4] X. Mu, et al., Appl. Sci. 10, 1538 (2020).

[5] T. Ren, et al., J. Appl. Phys. 125, 230901 (2019).

[6] Z. Wang, et al., Opt. Lett. 41, 4146–4149 (2016).

[7] Y.C. Jun, et al., Opt. Express 17, 7479 (2009).

[8] N. R. Verhart, et al., Opt. Express 22, 19633 (2014).

[9] M. I. Davanco, et al., Opt. Express 17, 10542 (2009).

[10] L. Liebermeister, et al. Appl. Phys. Lett. 104, 031101 (2014).

[11] D. Andrés-Penares, et al., Commun. Mater 2, 52 (2021).

POSTER: Designing Moiré Patterns by Twist, Strain or Bending.

Presenter

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Abstract

Experiments conducted on two-dimensional twisted materials have revealed a plethora of moiré patterns with different forms and shapes. Typically, the formation of these patterns is attributed to the presence of small strains in the samples, which usually arise during the fabrication process. In this work, we find that the superlattice structure of such systems critically depends on the interplay between twist and strain. Specifically, for systems composed of honeycomb lattices, we demonstrate that this interplay can lead to the formation of almost any moiré geometry, even when each lattice experiences only slight distortion. Consequently, we illustrate that under strain, the moiré Brillouin zone assumes the form of a primitive cell that adjusts according to the geometry of the strained moiré vectors. Furthermore, we elucidate the formation of nearly perfect one-dimensional moiré patterns in twisted bilayer systems. As a criterion for such a transition, we establish a simple relationship between twist, strain, and the material-specific Poisson ratio. This induced one-dimensional behavior is characterized by two periodicities, which are typically incommensurate. Our results provide explanations for the complex patterns of one-dimensional channels observed in low angle twisted bilayer graphene systems and twisted bilayer dichalcogenides. We also identify the conditions that allows the formation of hexagonal moiré patterns arising solely from shear or biaxial strain, thus presenting the possibility of engineering moiré patterns exclusively through strain. Moreover, we investigate the electronic properties within these moiré patterns and observe that strain tends to suppress the formation of flat moiré bands, even in strain-induced hexagonal patterns analogous to those obtained through only twist.

POSTER: Quadratic optical responses of Rashba surface states

Presenter

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Abstract

Crystal surfaces offer different symmetry properties from the bulk. For example, inversion symmetry is broken at the surface, allowing for Rashba spin-orbit coupling even in centrosymmetric crystal structures. As a result, second order optical responses, which require inversion symmetry breaking, take place at the surface of materials where it would not be expected. Here we analyze the interplay of quadratic optical responses and spin-split surface states. One prototypic material surface which exhibits this effect is Au(111), where the Rashba surface states are well separated from the bulk. In this work we report the k-resolved charge and spin second order photoconductivities calculated for the surface states. This is then compared with the analytic expressions calculated using the Rashba model including a hexagonal warping term [1], which reflects the C_{3v} symmetry of Au(111). The inclusion of the latter term is required in order to allow photocurrents flowing in the surface plane. As a second case study we consider $\text{Ti/Si}(111)$, which is a semiconductor with no bulk contribution to the photocurrent. The system hosts spin-split surface states that can be populated through hole or electron doping. Estimation of the current is given in this system for different values of the Fermi level for realistic experimental conditions. Our results show that the generated photocurrents should be measurable with current experimental techniques.

[1] L. Fu, Phys. Rev. Lett. 103, 266801 (2009)

POSTER: Unidirectional Ray Polaritons in Twisted Asymmetric Stacks

Presenter

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Abstract

The emergence of a vast repository of van der Waals (vdW) materials supporting polaritons – light coupled to matter excitations – offers a plethora of different possibilities to tailor electromagnetic waves at the subwavelength-scale. In particular, the development of twistoptics – the study of the optical properties of twisted stacks of vdW materials – allows the directional propagation of phonon polaritons (PhPs) along a single spatial direction, which has been coined as canalization. Here we demonstrate a complementary type of nanoscale unidirectional propagation that naturally emerges thanks to twistoptics: unidirectional ray polaritons (URPs). This natural phenomenon arises in two types of twisted hyperbolic stacks: homostructures of MoO_3 and heterostructures of MoO_3 and Ga_2O_3 , each with very different thicknesses of its constituents. URPs are characterized by the absence of diffraction and the presence of a single phase of the propagating field. Importantly, we demonstrate that this ray behavior can be tuned by means of both relative twist angle and illumination frequency variations. Additionally, an unprecedented “pinwheel-like” propagation emerges at specific twist angles of the homostructure. We show that URPs emerge due to the twist between asymmetrically stacked biaxial slabs, while the shear effect in monoclinic Ga_2O_3 is of minor importance. Our findings demonstrate a natural way to excite unidirectional ray-like PhPs and offer a unique platform for controlling the propagation of PhPs at the

nanoscale with many potential applications like nanoimaging, (bio)-sensing or polaritonic thermal management.

POSTER: Evidence of photo-accelerated aging of two-dimensional lead halide perovskites in ambient air leading to faster crystal decomposition with degraded photoluminescence

Presenter

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Abstract

Two-dimensional halide perovskites are promising for advanced photonic, optoelectronic, and photovoltaic applications. However, their long-term stability is still a critical factor limiting their implementation into further commercial applications. Here, we present an environmental stability analysis of $\text{BA}_2(\text{MA})_{n-1}\text{Pb}n\text{I}3n+1$ ($\text{BA}=\text{C}_4\text{H}_{12}\text{N}^+$, $\text{MA}=\text{CH}_6\text{N}^+$) two-dimensional perovskites with the lowest quantum well thicknesses of $n=1$ and $n=2$, after one year of aging under ambient humidity, oxygen content, and light conditions. Their structural, optical, and surface chemical changes were characterized by micro-photoluminescence, micro-Raman, and X-ray photoemission spectroscopy techniques. Both crystal phases ($n=1,2$) degraded similarly, resulting in the removal of organic components and crystal decomposition into PbI_2 , Pb oxides and Pb hydroxides. However, we have found a significant difference between their aging under ambient light and dark conditions, affecting their degraded morphology and photoactivity. We demonstrate that light is the most critical external factor accelerating 2D perovskite degradation processes in ambient air and thus affecting their long-term stability.

POSTER: Interaction of ultra-broadband fs-laser pulses with 2D materials

Presenter

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Abstract

Atomically thin transition metal dichalcogenides (TMDCs) display unique optical and electrical properties upon illumination with femtosecond (fs) laser pulses. In turn, such spatially and temporally confined light-matter interaction gives rise to new physical mechanisms that hold great potential for optoelectronic and photonics applications.

In this work, we investigate the interaction of ultra-broadband fs-laser pulses with atomically-thin TMDCs. To this end, we use a hybrid microscopy/spectroscopy arrangement combined with a d-scan layout. Our house-made microscope allows us to locate, image and characterize the thickness of flakes with single atomic layers of MoS₂. Subsequently, we collect spectra that result of the interaction of fs-laser pulses (650-1050 nm, 7.9 fs) with the identified monolayers. In particular, we use second-harmonic generation (SHG) to fully characterize few-cycle laser pulses using the so-called d-scan method. Our d-scan data consist of false-color maps of the SHG signal as a function of wavelength (x-axis) and of a controlled amount of optical dispersion (y-axis). The SHG signal is large enough to be recorded with standard spectrometers. Using a house-made algorithm, we retrieve the full information of the laser pulses, i.e. both laser intensity and phase in the temporal and spectral domains. The validity of our results is confirmed by comparing the results obtained using a 2D TMDC with those measured using a commercially available 10 μm -thick BBO crystal.

Additionally, to exploiting SHG for laser pulse characterization, we investigate nondegenerate optical processes that result from the interaction of fs-laser pulses with MoS₂ monolayers. Remarkably, we use a single ultra-broadband fs-laser source to originate said nondegenerate processes. Due to the inherent lack of phase matching requirements in atomically-thin materials, our spectra simultaneously illustrate signals linked to SHG, sum-frequency generation, four-wave mixing and nonlinear photoluminescence.

POSTER: Electronic band engineering in 3d intercalated transition metal dichalcogenides: Co_{1/3}TaS₂ and Fe_{1/3}TaS₂

Presenter

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Abstract

The electronic structure of chiral magnetic materials with noncollinear spin textures is promising for spintronic applications. The 3d intercalated transition metal dichalcogenides (3d I-TMDCs) represent a class

of intercalated layered materials that possess rich magnetic phases due to the localized magnetic moment of intercalants. Recently, the magnetic 3d I-TMDCs have been re-examined under the framework of topological physics. The antiferromagnet $\text{Co}_1/3\text{TaS}_2$ and ferromagnetic $\text{Fe}_1/3\text{TaS}_2$ have attracted considerable attention as potential noncollinear spin textures and topological band crossings were linked to the giant anomalous Hall effect observed in the compound. Here, we present a comprehensive suite of electronic structure studies on both $\text{Co}_1/3\text{TaS}_2$ and $\text{Fe}_1/3\text{TaS}_2$ using angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT). We show that bands in $\text{Co}_1/3\text{TaS}_2$ are more dispersive than their counterparts in $\text{Fe}_1/3\text{TaS}_2$, resulting in markedly different Fermi wavevectors. The comparison with TaS_2 suggests that the intercalation of Co atoms strongly modifies the electronic structure of $\text{Co}_1/3\text{TaS}_2$. Our ab initio calculation, consistent with experimental results, suggests strong hybridization between Ta- and Co or Fe-derived states near the Fermi level. Interestingly, the intercalated system exhibits a Kagome-like electronic structure in the Fermi surface with triangular pockets centered at K-points and the corner touching at the M high symmetry points. Intercalated TMCD systems offer a great opportunity to explore the rich physics associated with magnetic ordering and electronic structure in low-dimensional systems.

POSTER: Ultrafast magnetic field induced by anisotropy in carbon nanotubes irradiated by intense laser fields

Presenter

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Abstract

Carbon nanotubes exhibit remarkable responses to intense laser fields, revealing their unique optical and electronic properties. A notable nonlinear response is high-order harmonic generation, where the laser field drives the emission of harmonics with frequencies that extend up to the extreme UV regime. These responses are influenced by factors such as the diameter of the nanotube, chirality, or the intensity and wavelength of the driver. This contribution focuses on an unexpected result of the anisotropy of the nonlinear optical response of carbon nanotubes, inherent to their chirality. Indeed, we theoretically demonstrate that, upon irradiation with an intense linearly polarized laser pulse along the axial direction, chiral nanotubes exhibit an azimuthal current that is absent in achiral species. This current induces a magnetic field parallel to the axis of the nanotube that radiates like a loop antenna, see figure. Therefore, the total harmonic response of chiral nanotubes consists of two contributions, with polarization directions parallel and normal to the nanotube axis, depending on the geometry of the radiating current, axial or circular, respectively. Our results also shown that the response induced by the anisotropy of the target is greater for higher harmonic orders, in agreement with the results found for graphene in previous works. Furthermore, it is also observed that the optical response is highly influenced by metallicity, since the

efficiency results of the same order of magnitude in both the axial and azimuthal directions for semiconducting species, while for metallic species the response in the axial direction is several orders of magnitude greater than in the azimuthal. Understanding the complexities of carbon nanotube interactions with intense laser fields, particularly in the context of high-order harmonic generation, holds promise for applications ranging from ultrafast photonics to advanced optoelectronic devices.

POSTER: NEXT-BOLD: Synthesis and characterization of single molecule detectors for Ba²⁺ capture towards the background-free detection of neutrinoless ?? decay

Presenter

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Abstract

Over the course of have a century now, there has been an interest in solving a fundamental problem in physics involving the asymmetry of matter and antimatter in the universe.¹ One theory being tested is whether neutrinos are Majorana particles and therefore such a situation could explain the asymmetry.² The NEXT collaboration has been working on systems and experiments that could lead to the observation of a neutrinoless ?? decay of ¹³⁶Xe. Previous and current efforts are with experiments such as NEXT-100.³ Incorporating a single molecule indicator would provide a background-free detection of the neutrinoless double ? decay and improve our sensitivity to well beyond a half-life of 10²⁸ years. Our part in the collaboration (NEXT-BOLD) is to construct a system incorporating the molecular sensor and optics to capture and tag the ¹³⁶Ba²⁺ resulting from the decay of ¹³⁶Xe. We have previously investigated fluorescent bicolor indicator (FBI) molecules with a variety of techniques (LT-STM, XPS) for Ba capture.⁴ Recently, we have tested a new batch of fluorescent molecules such as NAPH3 (schematic in the figure). The current goal for such molecules is to have a clean “off” behavior in their free state and “on” when interacting with Ba²⁺. For NAPH3, preliminary results suggest chelation of Ba²⁺ when NAPH3 is deposited on quartz by evaporation. Differences in emission signal upon laser excitation of NAPH3 suggest an off-on behavior by the molecules. More work is needed to verify the efficiency of NAPH3 and other potential candidate molecules as single ion sensors using surface science techniques such as XPS and STM. This could mean a step forward in realizing a background-free measurement for the search of neutrinoless double beta decay and single ion sensing on surfaces in general.

1 Sakharov, D. *Sov. Phys. - Uspekhi* 34, 392–393 (1991)

2 Majorana, E. *Phys. Part. Nucl.* 34, 124–131 (2003)

3 Mistry, K. *et al. J. Instrum.* 19, (2024)

4 Herrero-Gómez, P. *et al. Nat. Commun.* 13, 1–11 (2022)

POSTER: Study of the exfoliation of two-dimensional Cu-doped TiSe₂

Presenter

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Abstract

Materials with thicknesses ranging from a few nanometers to a single atomic layer present unprecedented opportunities to investigate matter properties restricted to the two-dimensional plane. One of the most studied two-dimensional materials are the so-called transition metal chalcogenides. Among these materials, titanium diselenide (TiSe₂) and its derivatives stand out for their well-known physical properties, however, there are currently difficulties in their application. Jurelo et al. [1] studied through density functional theory (DFT) calculations the effect of copper (Cu) intercalation on the structural, vibrational and electronic properties of TiSe₂, observing that it exhibits properties of a high-temperature superconductor. Generally, the synthesis of two-dimensional TiSe₂ is performed by chemical vapor deposition, but to overcome the complexity and cost of this process, Rosa et al. [2] developed a method that consists of synthesizing and isolating 2D sheets from 3D Cu_xTiSe₂ crystals, through a solvothermal exfoliation process using hydrazine (N₂H₄) as a solvent.

With the goal of understanding how N₂H₄ influences the exfoliation of TiSe₂, we perform DFT simulations on TiSe₂, Cu_xTiSe₂ systems and their interaction with N₂H₄. In addition to analyzing the electrical and structural properties at the atomic level, we perform nudged elastic band calculations were performed to study the activation energy for the diffusion of Cu adsorbed on TiSe₂. Our results, consistent with those previously reported [1], reveal a favorable interaction between the N atoms of N₂H₄ and the Se atoms in TiSe₂. We also observed that the intercalation of N₂H₄ increases the separation between the TiSe₂ sheets, which decreases the van der Waals interaction between them and facilitates the exfoliation process in the 3D material. These effects are enhanced by the presence of copper in the Cu_xTiSe₂ structure, since N₂H₄ also interacts favorably with Cu atoms.

Phys.Chem.Chem.Phys., 20, 27011.

Alvaro Rosa, Thesis in Physics, UNRC (2021)

Scanning probe microscopies: a tool to understand and fabricate materials for future electronics (DFMC-GEFES) / Microscopías de sonda de barrido: una herramienta para entender y fabricar materiales para la electrónica del futuro (DFMC-GEFES)

Organiser

Héctor González Herrero (UAM) Daniel Martín Jiménez (ICMAB) Ana Pérez Rodríguez (U Salamanca)

Invited speakers

Daniel Ebeling (Universidad Justus Liebig, Gießen, Germany) Fabian Schulz (CIC nanoGUNE) Carmen Munuera (Instituto de Ciencia de Materiales de Madrid) Marc González Cuixart (Catalan Institute of Nanoscience and Nanotechnology), Sara Barja (University of the Basque Country) Eider Berganza (Instituto de Ciencia de Materiales de Madrid) Aitor Mugarza (Catalan Institute of Nanoscience and Nanotechnology) Niklas Friedrich (University Regensburg)

Symposium abstract

In recent years, improvements in the miniaturization and assembly processes of matter, as well as the use of novel chemical species, have placed nanotechnology as a major producer of new materials: customized organic molecules, nanowires, 2D materials and materials for energy, among others. These new materials are expected to be part of future electronic devices addressing some of humanity's current challenges, such as electronic efficiency, energy storage, climate change and disease control. Scanning probe microscopies (SPM) play a key role in the characterization and fabrication of these materials. These techniques provide valuable information at the nanometer scale about the structure and physical properties of materials. It also enables structure-property correlations, which is crucial for understanding the behavior of materials and is a source of inspiration for the design of new ones with specific properties. In addition, SPM studies on materials can be performed in situ on working devices, such as transistors, photodetectors or batteries. This symposium will cover SPM works for the production, characterization and test of materials for future electronics.

En los últimos años, las mejoras en los procesos de miniaturización y ensamblaje de la materia, así como el uso de especies químicas novedosas, han convertido la nanotecnología en una gran productora de nuevos materiales: moléculas orgánicas personalizadas, nanocintas, materiales 2D y materiales para la energía, entre otros. Se espera que estos nuevos materiales formen parte de los dispositivos electrónicos del futuro y que ayuden a resolver algunos de los retos actuales de la humanidad, como la eficiencia electrónica, el almacenamiento de energía, el cambio climático y el control de enfermedades. Las microscopías de sonda de barrido (SPM) desempeñan un papel fundamental en la caracterización y la fabricación de estos materiales. Estas técnicas proporcionan información valiosa a escala nanométrica sobre la estructura y las propiedades físicas de los materiales. También permiten establecer correlaciones estructura-propiedades, lo que resulta crucial para comprender el comportamiento de los materiales y sirve como inspiración para el diseño de otros nuevos con propiedades específicas. Además, los estudios SPM sobre materiales pueden realizarse in situ en dispositivos en funcionamiento, como transistores, fotodetectores o baterías. Este simposio incluirá trabajos de SPM para la producción, la caracterización y el test de materiales para la electrónica del futuro.

List of abstracts at the symposium

Towards correlative SPM and synchrotron-based studies at ALBA

1st author

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Abstract

Characterizing material's properties at the atomic scale requires the combination of multiple techniques that provide complementary insights. However, the characterization of surface properties of bulk materials, or 1D/2D materials must be carried out in ultra-high vacuum (UHV) conditions, challenging the multitechnique approach. In this case, the correlation among the different properties can be carried out at different levels. At the most simple level, assuming sample reproducibility and homogeneity, different samples can be used for each technique. Advancing to a higher degree of correlation involves transferring the same sample between instruments without breaking UHV, overcoming reproducibility issues but still facing the ones related to heterogeneity. To tackle this, one can combine UHV transfer, microscale probing, and colocalization to probe the same region of a sample with different techniques. Our group, in collaboration with ICMAB and ALBA, is currently developing infrastructure for correlative studies at the micro and nanoscale. This initiative is a follow-up of a joint effort with the BOREAS beamline at ALBA to couple a STM, which fostered collaborations for atomic-scale structure correlations with electronic and magnetic data [1-6]. In this presentation I'll show some representative highlights. Our ongoing initiative involves establishing the SPM Platform at ALBA, facilitating correlative measurements with 5 SPMs and different beamlines. I'll introduce the capabilities of the infrastructure, and the correlative studies that will be accessible.

- [1] M. C. Cuxart et al. ACS Nano 14, 6285–94 (2020).
- [2] M. Ormaza et al., Nano Lett. 16, 4230–35 (2016); L. Fernandez et al., Nanoscale, 12, 22258-22267 (2020).
- [3] S. O. Parreiras et al., Small 17, 2102753 (2021).
- [4] A. Lerch et al., J. Phys. Chem. C 121, 25353–63 (2017).
- [5] E. Bartolomé et al., Solid State Phenom. 257, 219–22 (2016); J. Phys. Chem. C 124 13993-14006 (2020); Adv. Mater. Interfaces 2300146 (2023).

Engineering a spin-orbit bandgap in graphene-tellurium heterostructures

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Abstract

The spin-orbit interaction (SOI) plays a pivotal role in shaping the electronic properties of materials, especially in the context of graphene-based heterostructures. In these systems, the interplay between the intrinsic SOI and external factors, such as heavy elements or intercalated species, can be strategically manipulated to induce and control unique electronic phenomena.

In this work, we report on a combined scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and Angle Resolved Photoemission Spectroscopy (ARPES) study on a new superstructure when Te is evaporated on graphene over Ir(111) [1]. Notably, a significant bandgap at the Dirac point is revealed at room temperature, rendering graphene nearly charge-neutral and allowing for the tuning of the Fermi level into the gap as a function of the Te coverage. The origin of the bandgap has been attributed to a substantial intrinsic SOI, presenting promising possibilities for electronic and spintronic device applications based on graphene/Te heterostructures.

[1] B. Muñoz Cano, *et al.*, arXiv:2311.16792.

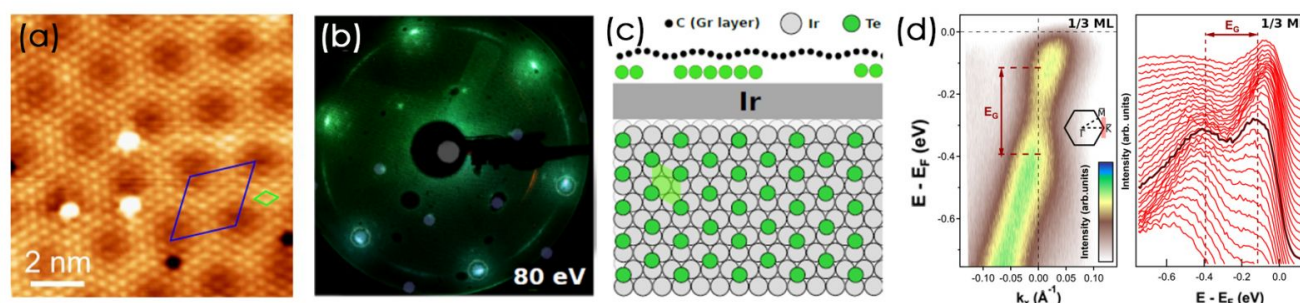


Figure 1: (a) High resolved STM image ($V_b=2$ V, $I_t=0.35$ nA). The moiré pattern unit cell of gr/Ir(111) and the one created by the intercalated Te are depicted in blue and green, respectively. (b) LEED pattern showing a pure $(\sqrt{3} \times \sqrt{3})R30^\circ$ reconstruction, described by the real space model in (c). (d) ARPES spectrum at K point of the Gr/Te/Ir(111) heterostructure and the corresponding Energy Distribution Curves evidence the gap opening at the Dirac point.

Fe coordinated N-doped graphene nanoflakes for NO₂ sensing

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Abstract

The versatility and precise control that on-surface synthesis provides has turned carbon nanoarchitectures into appealing systems for nanoelectronics, catalysis and sensing applications. Some ways to modify the electronic properties of graphene-like systems are reducing dimensionality in one direction by creating graphene nanoribbons or modifying the structure by chemical functionalization, pore formation or doping. These modifications hold potential for sensor development, with pores or dopant atoms serving as

anchoring sites for small analytes. Here, we study the growth of nitrogen doped graphene nanoflakes (N-GNFs) on Au(111) using scanning tunneling microscopy (STM) and high resolution X-ray photoelectron spectroscopy (XPS). Fe coordination and the effects of NO₂ exposure are characterized by XPS and near edge X-ray absorption fine structure (NEXAFS).

After triggering Ullmann coupling of N-GNFs molecular precursors by annealing at 200°C and the cyclodehydrogenation at 380°C, the N 1s core level shows a conversion of the original monomer with four pyridinic N into a periodic structure with 2 graphitic and 2 pyridinic N atoms. This results in the unexpected formation of a polymeric structure of periodic 3D N doped-GNFs, which could embed periodic Fe atoms. In fact, upon co-deposition of N-GNFs molecular precursors and FeBr₂ and further annealing, we observe a change in the N 1s core level suggesting the coordination of pyridinic N atoms with Fe. The exposure of the Fe coordinated N-GNFs to 50 L of NO₂ demonstrates an efficient interaction between Fe and NO₂ molecules. This interaction is manifested as a lowering of the first resonance in the N K-edge, a reduction of the intensity of the N-Fe component in the N 1s core level and 1 eV shift of the Fe L3-edge signal in NEXAFS. Our study paves the way to use 1D functionalized graphene-like materials for selective ion and gas sensing.

An Atomic-Scale Perspective on the Electrode-Electrolyte Interface

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Abstract

A fundamental understanding of processes at the electrode-electrolyte interface is crucial for developing optimized materials for sustainable energy production. However, obtaining a comprehensive atomic-scale picture of the chemical properties of surfaces, and their correlation to macroscopic catalytic performance, remains challenging. This difficulty is due to the complexity of real catalytic systems and the scarcity of experimental techniques capable of providing detailed insights—from single-molecule interactions to operando conditions—into the catalytic processes.

In this presentation, I will use two examples to illustrate the importance of atomistic studies on model electrocatalytic systems for understanding structure-function relationships and reaction mechanisms.

First, I will discuss the local properties of point defects in transition metal dichalcogenide semiconductors (MX₂, where M = transition metal, X = chalcogen) that are considered active sites for the hydrogen evolution reaction (HER). By integrating 4K scanning tunneling microscopy and spectroscopy (STM/STS) with non-contact atomic force microscopy (nc-AFM), our investigations have identified substitutional oxygen as a predominant point defect [1,2], which effectively suppresses deep in-gap states typically associated with chalcogen vacancies, previously thought to mediate HER. These findings underscore the critical role of local properties in determining material functionality for hydrogen production, thus influencing the underlying reaction mechanisms.

Second, I will introduce our custom experimental setup, which enables comprehensive characterization of the structural, chemical, and electrochemical properties of the same sample. This setup facilitates the transfer of electrodes from ultra-high vacuum conditions, ideal for surface science tools, to an electrochemical cell in an inert atmosphere. Employing this approach, we investigated potential-induced transformations on the Au(111) surface, operating as an electrode during the oxygen evolution reaction (OER). This study monitors the chemical changes through ex-situ X-ray photoemission spectroscopy. Our findings provide insights into how various electrolyte ions influence surface electro-oxidation, offering valuable information for optimizing catalytic performance. [*,**]

[1] Barja *et al.*, Nat. Comm. 10, 3382 (2019), [2] Schuler *et al.*, PRL 123, 076801 (2019)

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A new versatile Atomic Force and Optical Microscope with X-Ray access as nanoLab

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Abstract

Atomic Force Microscopy (AFM) techniques have revolutionized Nanoscience, allowing to perform a variety of experiments -imaging, characterizing and even manipulating- on a nanometer scale. AFM transcends its conventional role as a mere microscope, indeed it is considered a “nano lab on the tip” [1]. Despite its extensive use and multifaceted capabilities, AFM is beset by several inherent limitations. In particular, although AFM can measure many physical properties and can thus access a wealth of material properties on the nanoscale, its true spectroscopic capabilities are still limited.

The main goal of the present talk is to present our recently approved “Prueba de Concepto Project”, whose goal is to design, fabricate, and test the validity of a novel AFM-based equipment with optimal performance both as AFM and as high-performance optical system. The main challenge will be to allow for high numerical aperture access for optical characterization, in particular Raman Scattering (RS), as well as parallel/front view access for tip-enhanced RS and X-Ray-Scattering applications; while still maintaining high rigidity and low noise and low drift in AFM applications. The system will be modular using infinitely corrected objectives to have a collimated beam path that allows for high resolution optical microscopy of the tip-sample region that is being characterized also by AFM techniques. In addition to optical techniques, we aim to expand the capabilities of this modular AFM system to include X-ray Scattering (SAXS), Grazing-Incidence Small-Angle X-ray Scattering (GISAXS), and other related methodologies. The design's modularity inherently simplifies the fusion of AFM with these X-ray techniques, unlocking new possibilities for comprehensive nanoscale characterization. The talk will of course be open for possible discussions, suggestions and collaborations.

[1] E. Meyer et. al., Scanning Probe Microscopy: The Lab on a Tip, Springer 2004.

Insights into 2D-based Devices via operando Scanning Probe Microscopy

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Abstract

Two-dimensional (2D) van der Waals materials have shown great potential for integration as components in electronic devices due to their unique electrical and optical properties. Understanding the local behavior of these devices, often dominated by highly localized phenomena, is crucial for advancing their application. A critical aspect of this understanding is the material-metal contact, which significantly impacts device functionality and efficiency by influencing charge injection into the semiconductor materials via the contact metal.

In this talk, I discuss our recent approach to systematically study 2D-based devices under operando conditions using scanning probe microscopy (SPM). Our primary focus has been on investigating the contact between the electrode and 2D material to obtain local information about the potential barriers. By employing a two-terminal configuration, we can effectively probe the voltage drops along the device

through surface potential mapping. Based on the choice of electrode material, our findings reveal the ohmic and Schottky behavior of the contact, offering insights for optimizing 2D-based devices such as highly rectifying diodes or transistors with low contact resistance.

Additionally, we show how in-situ SPM manipulation can further enhance device performance.

This study aims to contribute to the advancement of 2D material-based electronics by providing valuable insights into the fundamental aspects of device operation and optimization strategies.

SCM and AM-KPFM of quantum devices at IMB-CNM

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Abstract

Atomic Force Microscopy (AFM) and related techniques enable the measurement of the topography of electronic devices with sub-nm precision in the Z direction. It often is also necessary to map the electrical properties of those same devices, for which a plethora of specialized modes of AFM exist. Here we discuss our application of AM Kelvin Probe Force Microscopy (AM-KPFM) and contact mode Scanning Capacitance Microscopy (SCM) to the characterization of electronic devices fabricated at the IMB-CNM (CSIC) and the University of Valladolid. The realization of single-electron transistors is a crucial step in the context of our push towards semiconductor-based spin qubits. AFM-based techniques are particularly well suited to imaging these planar devices. In particular, our measurements of the active area by SCM allow us to directly observe the depletion region of the source and drain areas, which serves as experimental validation of our space charge simulations, which in turn help us avoid carrier punch-through in the channel region. We also show our direct characterization of CVD-grown, multiple-junction, InP-In_{1-x}Ga_xP nanowire structures which are attractive for photovoltaic applications. Distinguishing the alternating P- and N-doped segments of these heterostructures requires resolution well below the micron scale, such as that provided by AM-KPFM. By using Electron Beam Lithography to affix the nanowires to the substrate, we can perform SCM measurements on them. Therefore, we are able to obtain topography, potential and capacitance maps, which are then contrasted with photoluminescence and Raman data.

Growth and atomic-scale insights into 2D materials beyond graphene

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Abstract

Inspired by the early example of graphene, most 2D materials developed in the following years have been isolated from naturally occurring layered materials. This approach, however, restricts the library of attainable materials. Synthetic growth methods can overcome this limitation by allowing custom choice of constituent elements, hence unlocking vast new possibilities for creating 2D materials with tailored properties. Borophenes, consisting on atomically-thin layers of elemental boron, are prominent examples of synthetic 2D materials, as they exhibit anisotropic metallicity and mechanical properties that expand the capabilities of conventional 2D materials [1]. Their intriguing multicenter boron-boron bonding results in the formation of a large number of 2D polymorphs (i.e., borophenes). These are typically grown on epitaxial substrates, in which interfacial interactions strongly influence the stabilization of a particular polymorph. It is therefore crucial to gain atomic-scale insights into these structures and explore suitable synthesis process for properties tailoring and creation of advanced borophene-based hetero-materials. In this talk, I will first review the exploration of borophenes since the early computational attempts to stabilize 2D boron structures, to the most recent advances towards device incorporation. Next, I will present how to grow borophenes by chemical vapor deposition, and the versatility of this method to fabricate functional borophene – hexagonal boron nitride heterostructures [2]. Atomic-scale insight into their structural, electronic and chemical properties is achieved thanks to a correlative study that makes use of scanning tunneling microscopy and synchrotron-based x-ray photoelectron spectroscopies [3]. Finally, I will assess whether the anisotropic structures of borophenes can be used as a unidirectional nano-template to steer molecular self-assembly, and compare it to the case of one-dimensionally corrugated hexagonal boron nitride [4]. These findings represent a step forward in the investigation these fascinating 2D materials, and exemplify the power of combining local-scale scanning probe microscopies with surface-averaged spectroscopic techniques.

[1] A. J. Mannix, et al., Nat. Nanotechnol. 13 (2018) 444-450.

[2] M. G. Cuxart et al., Sci. Adv. 7 (2021) 1-8.

[3] M. G. Cuxart et al., Carbon 201 (2023) 881-890.

[4] V. Chesnyak, et al., Small 2304803 (2023) 1-9.

Light assisted KPFM to study doping and surface defects in gallium nitride for power devices

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Abstract

Power devices play a crucial role in electronic systems and applications, facilitating essential functions such as the control and conversion of electrical power, switching or modulation. Among the various wide band-gap materials suitable for vertical power device development, GaN stands out for its exceptional attributes. GaN exhibits a high figure-of-merit, enabling operation at elevated temperatures while maintaining large blocking voltages and high critical electric fields. For achieving high breakdown voltage, device architectures include selectively p-type doped regions, and Mg ion implantation followed of rapid thermal

annealing emerge as preferred methods for this task. Nevertheless, implantation and annealing processes can result in defects and decreased acceptor activation. We report here on the characterization of Mg implanted GaN layers. Room temperature and 500 oC implantation is studied, with doses ranging from 2.5×10^{14} to 20×10^{14} cm⁻². Pulsed rapid thermal annealing at 1250 oC was used for Mg activation, with the sample's surface protected by a cap layer (10 nm SiN_x and 10 nm Al₂O₃). The surface morphology and the optoelectronic properties of the samples are investigated by ultraviolet light assisted Kelvin probe force microscopy (KPFM). Only one of the samples showed evidence of surface erosion. KPFM revealed surface electrical homogeneity in the rest of the samples, in contrast with findings from p-doped samples, where acceptor segregation is commonly observed. Above band-gap illumination (325 nm He-Cd laser) as a function of power enabled the study of the evolution of the surface photovoltage, providing information about carrier dynamics and trapping, surface band bending and doping. Acknowledgments: This project has received funding from the ECSEL Joint Undertaking (JU) under grant agreement No 101007229. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, France, Belgium, Austria, Sweden, Spain, Italy. Also financed by the European Union-NextGeneratonEU, PCI2021-121970/AEI / 10.13039/501100011033.

Surface charge dynamics in 2D materials and their relevance for AFM measurements

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Abstract

Two-dimensional (2D) materials have emerged as a promising platform for next generation devices. Thanks to their atomically thin structure and exceptional surface to volume ratio, they exhibit novel and exotic properties markedly different from those of their bulk counterparts. Given the nanoscopic scale of the problem and the correlation between morphology and physico-chemical properties, atomic force microscopy (AFM) techniques rise as an ideal tool to record morphology alongside electronic properties. A prevalent issue in the characterization of 2D materials with AFM is the inaccurate height determination from topography images, a problem which is enhanced when using dynamic modes, where the height tends to be overestimated. In this work, we show the existence of a dissipative Joule mechanism related with the surface charge dynamics that affects the measured height. This particular mechanism arises due to the presence of a finite surface conductivity, and is of particular relevance when 2D materials are supported on insulating substrates. To show this, we studied single-layer GO and rGO flakes, whose conductivities differ by several orders of magnitude, co-deposited on a silicon dioxide substrate in air at room temperature, and under UHV at varying temperature. These experiments allow us to verify that the Joule dissipation is long-ranged, and depends on the tip-sample surface potential difference, as well as on the temperature. Subsequently, we introduce a general model that allows to elucidate our observations, including the influence of the oscillating tip, and relating the increase in apparent height to a finite in-plane conductivity. Furthermore, our model provides a pathway towards understanding the effect of finite conductivity when determining the electrostatic properties of 2D materials with AFM.

Constructing organic nanomaterials molecule by molecule and deciphering on-surface reaction processes via chemical bond imaging

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Abstract

Constructing low-dimensional covalent assemblies with tailored size and connectivity is the key for applications in molecular electronics where optical and electronic properties of the quantum materials are highly structure dependent. We present a versatile approach for building such structures molecule by molecule on bilayer sodium chloride (NaCl) films with the tip of an atomic force microscope, while tracking the structural changes with single-bond resolution. [1] Covalent homo-dimers in cis and trans configurations and homo-/hetero-trimers were selectively synthesized by a sequence of dehalogenation, translational manipulation and intermolecular coupling of halogenated precursors (see Figure). Using scanning probe manipulation, we were also able to synthesize the structurally elusive molecule P3N3, an inorganic aromatic benzene analogue, which is difficult to obtain via traditional synthetic methods due to its high reactivity. [2] This work shows ways for synthesizing elusive molecules and organic nanoarchitectures, studying structural modifications and revealing pathways of intermolecular reactions. Moreover, possibilities for tweaking the bond imaging technique using torsional higher eigenmodes of qPlus sensors and an adaptive tip-sample feedback will be illustrated. [3,4] While torsional eigenmodes can be utilized to perform lateral force microscopy with single bond resolution an adaptive feedback mechanism is useful for imaging the molecules and the surface with atomic resolution in a single scan which allows precise determination of adsorption positions.

[1] Q. Zhong et al. Nature Chemistry 13, 1133 (2021)

[2] Q. Zhong et al. Angew. Chem. Int. Ed. e202310121 (2023)

[3] D. Martin-Jimenez et al. Nanoscale 14, 5329 (2022)

[4] D. Martin-Jimenez et al. (submitted)

On-surface synthesis of nanographenes with polyradical states

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Abstract

?-magnetism in carbon-based nanostructures offers a potential route towards molecular spintronics [PRL 102, 157 (2009)]. However, its realization relies on the precise control over the charge and spin state of the molecular building blocks. One promising candidate to achieve such level of control are triangulene nanographenes and their derivatives. Triangulene molecules are open-shell polycyclic aromatic hydrocarbons with a spin polarization arising from a sublattice imbalance in the finite-sized graphene flakes [PRL 62, 1201 (1989)]. Their electronic and magnetic properties can be engineered through, e.g., variation of their size or heteroatom doping.

Here, we show how a combination of solution and on-surface synthesis allows us to fabricate with atomic precision different spin-carrying nanographenes based on nitrogen-doped triangulenes. We characterize their structure as well as electronic and magnetic properties by a combination of low-temperature scanning tunneling microscopy, noncontact atomic force microscopy and Kelvin probe force microscopy, and rationalize our findings by extensive electronic structure calculations. Our results demonstrate how to modify the magnetic ground state, excitation energies, and polyradical character of triangulene-based nanographenes through precise control over their atomic structure.

The presented work is carried out in collaboration with the groups of Thomas Frederiksen at Donostia International Physics Center and Diego Peña at Universidade de Santiago de Compostela.

Spin Polarized Edge States in Chiral Graphene Nanoribbons

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Abstract

Following the discovery of strongly localized 1D states in zig-zag edges of graphene nanostructures [1,2], plenty of theoretical studies have predicted the existence of a spin splitting across the Fermi level of these states as a result of e-e interactions [3]. To date, experimental evidence of their spin polarization has been scarce and achieved through rather indirect approaches [4]. In this contribution, we present our results on graphene nanoribbons enclosed by chiral (3,1) edges [5] -thus with a high density of zig-zag segments- and synthesized directly on a GdAu₂ ferromagnetic monolayer on Au(111). The GdAu₂ enables the *in-situ* calibration of the spin sensitivity of bulk Cr-tips for spin-polarized STM [6], and stabilizes the magnetic moment of the chiral edges. In this way we are able to image the energy resolved spin-polarization of edge states in chiral graphene nanoribbons. We observe a spin splitting stemming from e-e correlations with spin polarization of about 10 %.

[1] Nakada, K. *et al. Phys. Rev. B* 54, 17954–17961 (1996)

[2] Ruffieux, P. *et al. Nature* 531, 489–492 (2016)

[3] Son, Y.-W. *et al. Nature* 444, 347–349 (2006)

[4] Wang, S. *et al. Nature Communications* 7, 11507 (2016)

[5] Li, J. *et al. Nature Commun.* 12, 5538 (2021)

[6] Bazarnik, M. *et al. Phys. Rev. B* 99, 174419 (2019).

Current rectification by unipolar hole transport in a free-standing designer graphene nanoribbon

1st author

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Abstract

Coherent electron transport through individual molecules is a vital technique to probe different quantum mechanical properties like energy level alignment, vibronic modes or spin states. Here, we investigate the electronic transport through on-surface synthesized graphene nanoribbons (GNRs) containing substitutionally embedded 2B-dimers by suspending individual GNRs in the junction between tip and substrate of a scanning tunnelling microscope (STM). A spin-polarized topological in-gap state can be induced inside 7-armchair GNRs by a single 2B-dimer and is detected in transport experiments by a localized Kondo resonance [1].

We find that the resonant transport through this state is unipolar with the singly occupied 2B-state being responsible for resonant hole tunnelling at either voltage polarity [2]. We observe large current rectification ($>10^5$) in the system, that we explain by asymmetries in the conditions for resonant transport between the two voltage polarities. As this condition depends on the tip-substrate separation, we are able to control the rectification ratio within several orders of magnitude by mechanically adjusting the spacing of tip and substrate. When tuning the bias voltage to resonant hole transport at both polarities, this allows us to invert the forward bias direction of the molecular rectifier.

Our results unravel the details of coherent and resonant hole tunneling through a molecular wire built from a single 2B-doped GNR, confirming their technological potential for single molecule electronics.

[1] N Friedrich, P Brandimarte, *et al.*, Phys. Rev. Lett., 125, 146801 (2020)

[2] N Friedrich, *et al.*, Advanced Materials, 2401955 (2024)

Unveiling the effects of curvature in magnetic domain-wall motion via Magnetic Force Microscopy

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Abstract

Magnetic nanostructure engineering for applications in data storage, sensing, or biomedicine, relies on the manipulation of stray fields and magnetic confinement through geometrical effects. The creation of 2D planar magnetic nanostructures in forms of magnetic stripes, dots or antidots has been intensively studied. One step further, the exploitation of effects related to curvature, has opened the field of curvilinear magnetism,¹ where the introduction of geometry-induced effects in curved magnetic wires and films allows breaking the symmetry towards the realization of chiral magnetic textures in magnetically soft materials, without the need of further interactions. It has been experimentally demonstrated that local curvature yields a pinning potential for domain walls (DWs),² while curvature gradient produces the opposite effect, acting as a driving force that prompts DW automotion.³ In this work, the competition between these two terms is experimentally assessed via Magnetic Force Microscopy measurements in a system which possessed these two ingredients: an Archimedean spiral (Figure 1a).⁴ With the aim to assess the dominant effects on the DW motion in systems with curvature and curvature gradient, we generate domain walls applying a saturating field that leaves the spiral in the onion state upon field removal (Figure 1b). Depinning fields of the generated DWs are experimentally determined by advanced 3D MFM modes. We demonstrate that they follow a decreasing trend with local curvature and an increasing trend with curvature gradient.

XMCD demonstration of 2D-Ferromagnetism on an atom-thick & extended 2D-MOF

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Abstract

Ferromagnetism is the collective alignment of atomic spins that retain a net magnetic moment below the Curie temperature, even in the absence of external magnetic fields. Reducing this fundamental property into strictly two-dimensions was proposed in metal-organic coordination networks, but thus far has eluded experimental realization. In this work, we demonstrate that extended, cooperative ferromagnetism is feasible in an atomically thin two-dimensional metal-organic coordination network, despite only ~5% of the monolayer being composed of Fe atoms. The resulting ferromagnetic state exhibits an out-of-plane easy-axis square-like hysteresis loop with large coercive fields over 2 Tesla, significant magnetic anisotropy, and persists up to $T_c \approx 35$ K. These properties are driven by exchange interactions mainly mediated by the molecular linkers that we explain with theoretical calculations. Our findings resolve a two-decade search for ferromagnetism in two-dimensional metal-organic coordination networks. <https://doi.org/10.1038/s41467-024-46115-z>

Surface Tension Measurements Using Atomic Force Microscopy on Micrometer-Sized Droplets

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Abstract

Surface tension plays a pivotal role in our understanding of wetting phenomena. While commercially available tensiometers and optical imaging techniques are effective for bulk liquid volumes, they fall short when dealing with extremely small sample sizes in the femtoliter range. In this study, we explore the use of Atomic Force Microscopy (AFM) as a promising tool for surface tension measurements. Previous research demonstrated the feasibility of performing Wilhelmy-like experiments with AFM by fabricating specialized “nanoneedle” shaped cantilever probes. By quantifying the capillary force between these probes and a liquid surface, surface tension can be calculated. However, we take a different approach. Instead of using custom nanoneedle tips, we employ standard pyramidal cantilever tips coated with a hydrophilic polyethyleneglycol-based polymer brush. This simple modification significantly reduces contact angle hysteresis for most liquids. Our methodology involves numerical simulations of liquid drops interacting with pyramidal or conical geometries. By correlating experimentally measured forces with these simulations, we

accurately determine surface tension. Our results for micrometer-sized drops align well with bulk tensiometer measurements for three test liquids (mineral oil, ionic liquid, and glycerol), with a maximum error of only 10%. Importantly, our approach eliminates the need for specially fabricated nanoneedle tips, streamlining complexity and reducing measurement costs. We believe this method holds great promise for precise surface tension characterization in microscale systems.

Stability of tobacco mosaic virus under high temperatures

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Abstract

Recently, biomolecules have gained interest for their potential use as templates for the synthesis of a wide range of nanomaterials. These molecules are stable under a wide range of conditions. They present well-defined structures and diverse biochemical functionalities which can be modified by genetic engineering. Among them, the tobacco mosaic virus (TMV) is a widely used biotemplate due to its rod-shape structure of 300nm long and 18nm thick and physicochemical properties, which allow it to withstand extreme conditions. Thus, TMV is an attractive option for the bottom-up fabrication of nanomaterials.

In this work, we study the evolution of TMV under high temperatures conditions. We show that this virus could resist temperatures as high as 175°C with low degradation. Over this temperature, the virus structure collapses rapidly, being fully degraded at 240°C. These results demonstrate and extend the high structural stability of TMVs, giving us more information about the feasibility of using these viruses for energy storage, catalysis, and sensor devices.

[1] K. Z. Lee, V. B. Pussepitiyalage, Y.-H. Lee, L. S. Loesch-Fries, M. T. Harris, S. Hemmati, K. V. Solomon, *Biotechnol. J.*, 16, 2000311 (2021).

[2] Y. Zhang, Y. Dong, J. Zhou, X. Li, F. Wang, *Molecules*, 23, 2311 (2018).

[3] J. M. Alonso, M. ? Górzny, A. M. Bittner, *Trends Biotechnol.*, 31, 530 (2013).

POSTER: Probing Interactions in Porphyrin-Graphene Materials: Insights from AFM and Raman Analysis

Presenter

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Abstract

The functionalization of graphene oxide (GO) and reduced graphene oxide (RGO) with diverse chemical species, especially those compatible with aqueous environments, have been extensively explored. Among these, porphyrins have emerged as promising candidates for creating new nanohybrid materials with unique photoactive properties, spanning applications in optoelectronics, sensing, and cancer therapy, among others.

In this work we study the interactions between protoporphyrin IX molecules and GO and RGO using various functionalization methods. By combining atomic force microscopy (AFM) with optical techniques such as fluorescence and Raman spectroscopy, we aim to establish a direct link between the nanoscale morphological, electronic, and optical characteristics of the resulting nanohybrids. Through this multidimensional analysis, we seek to gain deeper insights into the intricate interplay between the molecules and graphene-based materials.

POSTER: Atomic-scale visualization of multiferroicity in monolayer NiI₂

Presenter

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Abstract

NiI₂ is a newly discovered layered multiferroic material, opening the possibility of realizing monolayer multiferroic systems [1-3]. While earlier investigations into its properties have involved a variety of methods (e.g., scattering-based, and optical bulk techniques), these approaches face significant limitations when applied to 2D materials, and experiments at the atomic scale are needed to fully characterize the multiferroic order at the monolayer limit. To address this challenge, we use scanning tunneling microscopy (STM) supported by density functional theory (DFT) calculations to probe and characterize the multiferroic order in monolayer NiI₂. Moreover, using an external electric field we directly manipulate the multiferroic domains observed in monolayer of NiI₂. This method provides a clear demonstration of the magnetoelectric coupling within the material. These findings not only advance the understanding of multiferroic materials in 2D systems, but also open avenues for future applications in nanoscale devices where control over multiferroic domains is crucial.

[1] Mohammad Amini, et.al. "Atomic-Scale Visualization of Multiferroicity in Monolayer NiI₂," Adv. Mater. 2024, 2311342.

[2] Adolfo O Fumega, et.al. "Microscopic origin of multiferroic order in monolayer NiI₂," 2D Materials 9, 025010 (2022).

[3] Qian Song, et. al. "Evidence for a single-layer van der Waals multiferroic," Nature 602, 601–605 (2022).

POSTER: AFM showing hydrophobic/hydrophilic surface maps over lettuce leaves

Presenter

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Abstract

Lettuce is one of the most consumed vegetables in the world and gaining knowledge on its leaf surface features owing to its perishable nature during postharvest storage and contamination with human pathogens as reported in several studies. By implementing an array of analytical and microscopic techniques, such as electron and atomic force microscopy (AFM), Fourier Transform Infrared (FTIR) and Raman spectroscopy, we observed that Romaine lettuce leaf surfaces are chemically heterogeneous at the nanoscale with focus on leaf stomata and AFM measurement. In our AFM experiments we used a low force constant which allows the tip-sample system to remain in attractive regime where the interaction is due to the formation and rupture of liquid necks. This parameter is subsequently picked up in the frequency shift and can be directly related to wetting properties of the analyzed material hence enabling to obtain hydrophilic/hydrophobic surface maps as here shown for lettuce leaves. Different chemical and structural surface patterns were estimated for stomata and neighboring pavement cells which indicates the variable nature of leaf epidermal cells an their protecting cuticle. Both lettuce leaf surfaces are wettable by water which will be related to the occurrence of hydrophilic nano-scale, cuticle areas as shown in our AFM images of stomata and pavement cells.

POSTER: Olive leaf wettability: from nanoscale to macroscale with focus on trichomes

Presenter

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Abstract

Wetting is the ability of a liquid to be in contact with a solid surface, resulting from intermolecular interactions when they are brought together. A precise understanding of the composition-structure-function of many biological and bio-inspired interfaces is still an open issue, in particular for the case of bio-wetting. Here the macro-, micro-, and nano-scale features of olive leaf have been analyzed. The olive leaf surfaces evaluated have few trichomes in the adaxial side versus a high trichome frequency in the abaxial leaf side. By combining different techniques including goniometry, electron and atomic force microscopy, the surface of both plant materials has been found to be chemically (hydrophilic-hydrophobic) heterogeneous at the nanoscale. The ultra-structural pattern observed for epidermal pavement cells differs from the reticulate cuticle structure of trichomes, which shows that leaf surface areas may be substantially different despite being located nearby. Our study proves for the first time the nano-scale chemical

heterogeneity of a hair which may provide key functional properties to biological surfaces as discussed here for plants.

POSTER: Exploring thin films engineering techniques for organic electronics: fluorinated fullerenes and coronene

Presenter

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Abstract

The non-covalent self-assembly of at least two organic compounds in a solid with a well-defined stoichiometry and structure originates a co-crystal, which usually leads to physical-chemical properties different from those of the precursors. Therefore, co-crystal engineering techniques have emerged as one of the routes for the generation of new organic functional materials in molecular electronics [1]. Though commonly aromatic and planar molecules are used for co-crystals achievement, it has been shown more recently that, by solution-based processes, bulky acceptor molecules (as standard C60), can form co-crystals in bulk [2-3] with non-planar donors (as Corannulene, C₂₀H₁₀), through concave-convex π - π interactions. Our approach to obtain extremely thin films of donor/acceptor compounds, includes using stronger acceptors as diverse C₆₀F_x (x= 0, 18, 36, 48) and a flat donor molecule (Coronene, C₂₄H₁₂). The molecules are deposited by gas-phase sublimation in ultra-high-vacuum and the starting benchmark substrate is Au(111)/mica. Scanning probe microscopy (SPM) is used to show how the two molecular specimens arrange on the substrate as a function of the specific fullerene derivative and evaporation conditions. The experimental study presented here will be of relevance for understanding the initial stages formation of non-conventional donor/acceptor systems and the development of engineering techniques for the production of co-crystal thin films for molecular electronics applications.

[1] L. Sun et al. Adv. Mater. 31, 1902328 (2019).

[2] Y. Wang et al. Nanoscale 8, 14920 (2016).

[3] G. Gao et al. J. Am. Chem. Soc. 142, 2460 (2020).

POSTER: Characterizing wetting phenomena: from macro-, meso- to nano-scale

Presenter

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Co-presenter

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Abstract

Wetting of liquid drops on a solid surface is fundamental to many biological and industrial processes. Traditionally, wetting is characterized by contact angle measurements, which is the optically observed angle that a drop sitting on a surface assumes at the three-phase contact line. The precise value of the contact angle fundamentally depends on various nano-scale interactions that the liquid molecules experience with the surface and the surrounding atmosphere at the three-phase contact line. Nano-scale chemical and topographic heterogeneities of a surface profoundly affect macro-scale contact angle

measurements, which show a hysteresis with the value lying between the advancing and receding contact angle. While macroscopic wetting behaviour has been extensively studied, nano-scale wetting studies have been limited due to their challenging nature. In our work, we demonstrate that Atomic Force Microscopy (AFM) can be a valuable tool for characterizing the wetting of water on surfaces at the nano scale. By performing imaging in the “non-contact mode” with a phase-locked loop under a humid atmosphere, we show that the frequency shift of the cantilever oscillation is directly related to the nano-scale wetting property of the surface. We propose that this frequency shift is caused by the spontaneous condensation of liquid water necks when the AFM tip is close to the surface. Such a liquid neck would result in a capillary interaction force with the tip that would depend on the nano-scale contact angle of water with the surface. We tested this approach by characterizing gold surfaces functionalized with thiol, forming micro-scale patterns which served as a model surface. Using appropriate modelling, the nano-scale contact angle was obtained from AFM data and was compared with the macroscopic contact angle of the gold-thiol surface.

POSTER: Polarization-dependent photocurrent spectra and nanoscale characterization of 2D ReS₂ field effect transistors.

Presenter

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Abstract

Transition metal dichalcogenides (TMDCs) are a class of bidimensional semiconductors that have attracted a lot of attention in the last decade for their integration in optoelectronic devices due to their unique electronic and optical properties [1]. In particular, lots of efforts are focused on Rhenium disulphide (ReS₂) due to its low crystal symmetry, that leads to the emergence of dichroic optical and optoelectronic response [2,3]. To unravel the full potential of ReS₂, studies on its optoelectronic response as well as in the impact of the morphology of the layers on its electrical and electrostatic properties must be done. In this work we perform a thorough study, characterizing the morphological and electrostatic characteristics of single and multi-layer ReS₂ samples and extracting the polarization-dependent photocurrent spectra of few-layer ReS₂ photodetectors, both in room conditions and at cryogenic temperature (14 K). By measuring the polarization-resolved photocurrent spectra [4], we obtain a clear linear dichroic (by a factor 2) behaviour of the photocurrent and the modulation as function of the light polarization angle of three different excitonic transitions, X1, X2 and X3, matching the photoluminescence measurement. Moreover, Kelvin Probe Force Microscopy (KPFM) measurements were performed in few-layer thick samples and working devices, obtaining the work function dependence with the number of layers and the potential drop through the device, evaluating the contact resistance and carrier mobility within the layer. Our results show that ReS₂ is a promising candidate for optoelectronics, with large carrier mobility and a dichroic photocurrent behaviour suitable for devices that aim at exploiting symmetry dependent effects.

[1] S. Manzel et al, *Nature Reviews Materials*, 2, (2017).

[2] F. Liu et al., *Adv Funct Mater*, 26, 8, pp. 1169–1177, (2016),

[3] J. Wang et al. *Advanced Materials* 32.32 (2020):

[4] D. Vaquero et al., *2D Materials*, 11, 1, (2023)

POSTER: Magnetic Force Microscopy: a tool to understand the influence of the magnetic screening of 2D materials with potential applications in electronic devices

Presenter

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Abstract

The singular electronic and physical properties exhibited by two-dimensional (2D) layered materials have attracted increasing attention over the past decades as potential candidates for use in electronic devices [1,2]. In particular, the study of their magnetic behavior is crucial to understand and predict how an external stimulus such as a magnetic field could affect the device performance, as well as to predict the effect of the combination of these layered materials with a magnetic component on a hypothetical electronic device.

Magnetic force microscopy (MFM) constitutes a powerful technique sensitive to the interaction between a sharp magnetic tip and the stray field of a magnetic sample. This allows direct imaging of the magnetic domains present at the surface, combined with high spatial resolution at the nanoscale, very convenient for property-structure correlation studies [3, 4]. However, it is critical to consider possible artifacts that may be present when measuring such systems. In that sense, the combination of MFM and Kelvin Probe Force Microscopy (KPFM) [5] or the application of in situ magnetic fields are very useful tools for these studies.

In this work, few layers of various 2D materials with different electronic/magnetic properties have been positioned onto a ferromagnetic thin film by deterministic transfer. This has allowed us to study their effect on the magnetic signal as a function of their electronic and structural properties [6].

POSTER: Charge-transfer complexes for organic semiconductor thin film devices

Presenter

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Abstract

Charge-transfer complexes (CTCs), arising from an ordered mixed assembly of small conjugated molecules, typically an electron donor and acceptor, have emerged as a materials design strategy for developing organic semiconductors with novel electrical and optical properties far beyond the performance of single materials, avoiding more complicated synthesis procedures [1-3]. Here, we study the formation of a thin film co-crystal made of 2,7-bis(octyloxy)[1]benzothieno[3,2-b]-benzothiophene (C8OBTBTOC8) and 1,3,4,5,7,8-hexafluoro-tetracyanonaphthoquinodimethane (F6TCNNQ) and demonstrate their absorption in the near-infrared (NIR). Obtained from molecular beam deposition in UHV, the co-crystal formation is revealed and characterized by combining Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS), Atomic Force Microscopy (AFM), Kelvin Probe Force Microscopy (KPFM) and UV-vis spectroscopy.

[1] L. Sun et al. Adv. Mater. 31, 1902328 (2019).

[2] W. Wang et al. Chem. Eur. J. 27, 464 (2021)

[3] Y. Wang et al. Angew. Chem. Int. Ed. 57, 3963 (2018).

POSTER: Molecular sensors for individual Ba tagging: application in neutrinoless double beta decay experiments

Presenter

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Abstract

If neutrinos are their own antiparticles, a very rare nuclear process ($T_{1/2} > 10^{26}$ yr) called neutrinoless double beta decay can occur. An unambiguous observation of such decay would open a window to answer transcendental questions beyond the physics known today, like the Universe preference for matter over antimatter or the origin of neutrino masses.

To succeed, experiments looking for these decays need to work in a highly controlled and hard-to-reach background-free regime, for which the “barium tagging” technique is being developed, consisting in identifying the Ba^{2+} daughter ion generated in ^{136}Xe double beta decays.

Recent studies [1,2] profit from the atomic resolution provided by STM to study molecular sensors with the expected ability to trap individual Ba^{2+} ions inside a ton-scale chamber of Xe gas, achieving the zero-background regime that experiments need. By bringing surface science and particle physics together in this way we expect to obtain a new perspective onto the research developed by multiple groups worldwide.

In this study we present the results obtained for the molecular sensors called FBI-G2 (Fluorescence Bicolor Indicators) adsorbed on a Au(111) surface, studied by STM and STS.

Our findings are that depending on the isomer of the sensor, these molecules arrange in different geometries, and that this arrangement depends in turn on the molecular coverage, which can be controlled. We also report that monomers and dimers have different electronic structures, as their HOMO-LUMO gaps differ, and so are expected to do their fluorescent behaviors. This way, monomers and dimers could be distinguished by optical fluorescence setups.

Furthermore, we show that the proportion of monomers and dimers on the surface can be tuned by the deposition of ions such as Ba^{2+} or Fe^{2+} , as these ions break dimers into monomers, thought to happen due to the chelation of the sensors by these ions. This, together with the finding that the gaps for monomers and dimers differ, allows us to prove that FBI-G2 sensors provide an effective way to detect the deposition of ions for the eventual application in single ion detection experiments.



Advances and perspectives in the physics of liquid crystals (DFMC-GEFES) / *Avances y perspectivas en la física de cristales líquidos (DFMC-GEFES)*

Organiser

Alberto Fernandez-Nieves (UB - ICREA), Jose Manuel Romero Enrique (U Sevilla)

Invited speakers

Jordi Ignes-Mullol (U Barcelona, Spain)

Symposium abstract

Aside of their many technological applications, liquid crystalline materials continue to be the subject of intensive fundamental research. The past recent years have witness the discovery of new phases, including the twist-bend or the nematic ferroelectric phase. In addition, there has been progress in the control and mobility of topological defects, including skyrmions in cholesterics. Furthermore, active liquid crystals exhibit fascinating phenomenology, and colloidal partially-ordered materials continue to provide examples of unexpected and interesting physics. This symposium aims at showcasing these as well as other recent advances in the field to try and create synergies between researchers in Spain working with liquid crystals.

Además de por sus aplicaciones tecnológicas en dispositivos electrónicos, los cristales líquidos continúan siendo de gran interés en investigación fundamental. Así, en los últimos años se han observado experimentalmente nuevas fases como la twist-bend o nemática ferroeléctrica. Además, se ha avanzado en el control y movilidad de defectos topológicos, tales como skyrmiones en fase colestérica bajo campos eléctricos oscilantes. Finalmente, los cristales líquidos activos presentan una fenomenología fascinante más rica que sus versiones pasivas. Este Simposio pretende mostrar avances recientes en el campo y crear sinergias entre los distintos grupos que investigan sobre cristal líquido en España.

List of abstracts at the symposium

Control and symmetry breaking in active nematic liquid crystals.

1st author

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Abstract

Active liquid crystals are fluids whose microscopic constituents convert surrounding energy sources into mechanical work, leading to the emergence of long-range orientational order and seemingly disordered self-sustained flows. Most examples are found in living systems, such as bacteria colonies, cellular epithelia, or cytoskeleton structures. In this research, we will focus on the quasi-two-dimensional active nematic obtained through the in-vitro reconstitution of microtubules and kinesin molecular motors. This active fluid layer forms at the interface between an aqueous and an oil medium and is hydrodynamically coupled to both. The system is characterized by seemingly disordered flows and by the proliferation of semi-integer topological defects, in a regime called active turbulence. I will discuss different strategies to control this material, based either on tuning the interfacial rheology or in confining the active flows to microfluidic channels, and I will explain what we can learn from these fascinating out of equilibrium liquids.

Liquid crystal skyrmions in shear flows

1st author

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Abstract

Liquid crystal skyrmions are topologically protected configurations of the director field formed under confinement between two parallel plates. They can be distorted and displaced, for instance, using an oscillating electric field, but not easily destroyed. Because the medium is liquid, mass flows naturally emerge due to director relaxation and/or applied forces. In this presentation, we address the hydrodynamic effects of a flowing skyrmion in two different cells: Poiseuille-like flow (forced flow between stationary plates) and Couette-like flow (relative uniform motion of the plates). We use lattice Boltzmann simulations in GPU of a 3D domain and experiments to study the dynamics, deformations and stability of the skyrmions. We find that, in Couette-like flows, the skyrmion moves in inclined trajectories with respect to the direction of the plate motion, as a result of local changes in the fluid flow around the skyrmion. For Poiseuille-like flows, the skyrmion distorts and moves at a constant speed under small forcing while it is destroyed by shear under higher forcings. This study is relevant in future lab-on-a-chip applications of display and memory technologies.

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[1] R. C. V. Coelho, M. Tasinkevych, M. M. Telo da Gama. J. Phys.: Condens. Matter 34 034001 (2021).

[2] R. C. V. Coelho, H. Zhao, M. Tasinkevych, I. I. Smalyukh, M. M. Telo da Gama. Phys. Rev. Research 5, 033210 (2023).

Active nematic defects in flat and curved surfaces

1st author

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Abstract

Topological defects manifest as salient features of liquid crystals. They are regions where the underlying director field is undefined. When driven out of equilibrium via an energy input at the single particle level, these defects develop unique self-propelling dynamics and interactions. In this work, we explore the rich phenomenology of defects in active liquid crystals confined to surfaces of different topology and varying curvature. We image the active nematic via fluorescence confocal microscopy and extract the underlying director fields via our image analysis algorithms based on computer vision techniques [1]. We then identify defect positions and orientations to define order parameters for the set of active defects. In 2D flat-space experiments, we observe short-range anti-ferromagnetic alignment of $+1/2$ defects and a somewhat surprising ferromagnetic alignment mediated by the presence of $-1/2$ defects [2]. However, the system

does not develop any long-range or quasi-long-range order over time. The qualitative features of defect-defect correlations are found to be independent of defect density. In curved space experiments, we observe a clear preference for the orientation of defects and persistent long-range order detected on highly curved regions of toroidal surfaces [3]. This is a remarkable confirmation that curvature, and its gradients, have a major role in intrinsically biasing defect alignment. This is in stark contrast to random, isotropic defect orientations found in locally flat regions. We also quantify defect number fluctuations. Overall, our work explores the rich interplay between activity, topology and curvature in a liquid crystalline system and how topological defects fluctuate in number and interact, developing correlations and orientational order.

[1] P. W. Ellis, J. Nambisan, and A. Fernandez-Nieves, *Mol. Phys.*, 118, 9-10, e1725167 (2020).

[2] D. Pearce, J. Nambisan, P. Ellis, A. Fernandez-Nieves, and L. Giomi, *Phys. Rev. Lett.*, 127, 19, p. 197 801 (2021).

[3] Work in progress (2022-)

Investigations on the polar properties of the ferroelectric nematic phase

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Abstract

Ferroelectric phase transitions in crystalline solids have long been the subject of intensive research. In the case of liquid crystals, chiral smectic and columnar phases were the only systems in which such phenomena could be observed. This led the community to believe that the emergence of ferroelectricity required a certain degree of positional order. However, this notion has been proven to be untrue due to the discovery of the ferroelectric nematic phase, the system with the highest symmetry that can exhibit long-range polar order. Shortly after the ferroelectric nematic phase was discovered, the existence of an intermediate phase between the high-temperature nematic phase and the low-temperature ferroelectric phase was reported in some compounds, which turns out to be a splay-modulated antiferroelectric phase. Hence, it is often called splay nematic. Moreover, very recently, a handful of new ferro- and antiferroelectric phases have also been discovered in the phase sequence of new compounds boasting the ferroelectric nematic phase. The liquid crystal community is thus witnessing a "polar revolution", and there is a great interest to understand the physics of these systems, which could foster promising future applications. In this contribution, we will try to convey the utility of broadband dielectric spectroscopy to probe the polar properties of these materials, especially from a molecular point of view. Our investigations on various ferroelectric nematogens have revealed some universal features which will undoubtedly help to improve our understanding.

Modelling and simulation study of discotic liquid crystals using coarse-grained models

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Abstract

The exploration of computational modelling of discoid molecules is a central aspect of colloid and liquid crystal science, playing a fundamental role in the intelligent development of a wide range of functional materials. In this contribution, we present an adaptive interaction model capable of unravelling the intricate mesogenic behaviour of discoidal particulate fluids. Using a spherocylindrically symmetric model as a reference, several classes of particle interactions with anisotropy have been defined, which promote specific relative particle orientations, such as stacked, lateral, cross and T-shaped configurations. This approach opens avenues to systematically customise the liquid phase diagram of the discotics. With the models thus defined, Monte Carlo simulations have been run on a number of case studies to elucidate the correlation between the interaction topology and the occurrence of nematic, smectic and columnar stable phases. In addition, the simulations shed light on less common phenomena, such as cubic, uniaxial and biaxial columnar domains, showing the wide spectrum of mesophases that can be achieved by tailored interactions.

Nematic defect structures in solid tori

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Abstract

Topological defects in nematic liquid crystals are regions where the orientational order is lost. Defects can be generated by quenching the nematic liquid crystal from the isotropic phase through a Kibble-Zurek mechanism leading to the formation and eventual annihilation of defects. Depending on the boundary conditions imposed on the liquid crystal phase, defects can be unavoidable. For example, in a 2-sphere with tangential boundary conditions for the director field, the total topological charge of the defects must be +2, as required by the Poincaré-Hopf index theorem. The presence of defects in the ground equilibrium state is thus required. For the case of a nematic liquid crystal confined to solid tori with parallel anchoring conditions the total topological charge must be zero, so no topological defects are required and a defect-free doubly twisted structure is often observed. Nevertheless, if the liquid crystal is heated to the isotropic phase and cooled back to the nematic phase, stable defect structures consisting of ± 1 boojum defect pairs appear and are stable for as long as the nematic torus lives.

When applying magnetic fields to our nematic liquid crystal, the anisotropic building blocks will tend to align in the direction of the field. Our results show the formation of some kind of highly distorted Helfrich walls for the defect-free case and the case with defect pairs. Depending on the initial position of the defect pair, these walls can be moved around the torus. We also show the ability to generate two defect pairs in a controlled way by means of a temperature quench from the isotropic to the nematic phase in the presence of a magnetic field, highlighting how external fields can help control the otherwise largely uncontrolled defect structure that will result.

Tunable Bound states in continuum (BICs) in a liquid crystal wave-guide

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Abstract

This work reports the mode propagation in a waveguide whose both core and substrate are anisotropic. By applying a voltage to a liquid crystal (LC) waveguide structure, the orientation in the polar direction of the optical axis at the LC core can be tuned. This symmetry breaking phenomenon can lead to bound states in continuum (BICs) which are non-radiating which however are located in continuum[1]. These are interesting due to their very existence as confined modes and potential applications as filters and ultra-high quality resonators. It is a first ever evidence to demonstrate the effect of polar anisotropic symmetry breaking by electrically tuning the optic axis of the core which is a liquid crystal (LC) layer. From the theoretical modal spectroscopy, we observe the existence of switchable interferometric BICs in the antiguiding LC waveguide on a calcite substrate with polar anisotropic symmetry breaking. The position of the interferometric BIC can be tuned in the same system by applying an electric field. The aim of this work is to get first ever experimental evidence of the tunable leaky modes in an anisotropic core-substrate waveguide with misaligned optical axis orientation, followed by demonstrating the control of BIC existence by the variation of electric field and other optical parameters, for realizing the potential of active BIC-based photonic devices.

Mukherjee Samyabrata, Gomis-Bresco Jordi, Pujol-Closa Pilar, Artigas David & Torner Lluís, Topological properties of bound states in the continuum in geometries with broken anisotropy symmetry. Phys. Rev. A 98, 063826 (2018)

Orientational transition in nanobridges of nematic liquid crystals in slit pores

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Abstract

In this work, the morphology of nematic capillary nanobridges in slit pores separated by a vertical distance D will be characterised by Monte Carlo simulations for oblate molecules nematogen modelled by the Gay-Berne potential. Previous studies on droplets show that the molecules are arranged homeotropically at the nematic-vapour interface and form spherical droplets with an annular disclination located in their equatorial plane. In the presence of pores with attractive substrates that favour homeotropic anchoring, the formation of nanobridges characterised by anchoring angles that decrease with increasing particle-substrate interaction intensity is observed. When the orientational field in the nanobridge is analysed, the formation of an annular disclination of topological charge $+1/2$ located in the plane perpendicular to the z -axis that passes through the centre of mass of the nanobridge is observed for small D . However, when considering higher values of D , a change to a biaxial orientational profile within the nanobridge is observed, where now the annular disclination is arranged in a plane perpendicular to one direction of the xy plane. These results are indicative of the existence of an orientational phase transition for an intermediate D value between a uniaxial and a biaxial orientational configuration in the capillary nanobridge.

Materials and Methods for Quantum Technologies / *Materiales y Métodos para Tecnologías Cuánticas*

Organiser

Hermann Suderow (UAM) Edwin Herrera (UAM) Katerina Vaxevani (Nanogune) José Ignacio Pascual (Nanogune) Javier Aizpurua (DIPC)

Invited speakers

Angela Wittman (JGU Mainz) M. F. Goffman (CEA-Saclay, Université Paris-Saclay) J. Argüello (Universitat Politècnica de Catalunya)

Symposium abstract

Nowadays, research and advances in quantum technologies have a well-established role in the field of solid-state matter physics. For example, an increasing number of devices that utilize quantum effects benefit from the macroscopic quantum coherence. Its robustness to interference can be considerably improved by taking advantage of topological protection. Recent findings in band structure calculations show that there is an exploding number of materials that present topologically nontrivial states and/or exotic superconductivity. Furthermore, quantum variational eigenvalue methods have been developed to obtain minimum energy states in molecules and matter. Additionally, numerous experimental methods for the manipulation of these quantum states have been developed, as microwave spectroscopy combined with transport measurements. To augment the possibilities of such quantum materials, exploring the interaction of magnetism and superconductivity has been proven useful for the rapid advance of quantum technologies. The workshop will explore the properties of devices for quantum sensors and connect to recent developments in quantum computation.

The symposium invites contributions in fields such as:

- Non-trivial band structures of 2D materials and magnetic systems.
- 2D materials.
- Superconductivity.
- Manipulation of quantum states with microwaves.
- Molecular magnets.
- Hybrid structures and proximity-induced quantum phenomena.
- Quantum sensors.
- Quantum computation and algorithms.

Symposia supported by the Condensed Matter Physics Center (IFIMAC) and Condensed Matter Physics Department, Universidad Autónoma de Madrid.

Hoy en día, la investigación y los avances en tecnologías cuánticas tienen un papel bien establecido en el campo de la física de la materia del estado sólido. Por ejemplo, un número cada vez mayor de dispositivos que utilizan efectos cuánticos se benefician de la coherencia cuántica macroscópica. Su robustez a las interferencias se puede mejorar considerablemente aprovechando la protección topológica. Hallazgos recientes en cálculos de estructuras de bandas muestran que existe una enorme cantidad de materiales que presentan estados topológicos no triviales y/o superconductividad exótica. Además, se han desarrollado métodos de valores propios variacionales cuánticos para obtener estados de energía mínima en moléculas y materia. También, se han desarrollado numerosos métodos experimentales para la manipulación de estos estados cuánticos, como la espectroscopia de microondas combinada con mediciones de transporte. Para aumentar las posibilidades de tales materiales cuánticos, se ha demostrado que explorar la interacción del magnetismo y la superconductividad es útil para el rápido avance de las tecnologías cuánticas. El taller explorará las

propiedades de los dispositivos para sensores cuánticos y se conectará con los desarrollos recientes en computación cuántica.

El simposio invita a realizar contribuciones en campos como:

- *Estructuras de bandas no triviales de materiales 2D y sistemas magnéticos.*
- *Materiales 2D.*
- *Superconductividad.*
- *Manipulación de estados cuánticos con microondas.*
- *Imanes moleculares.*
- *Estructuras híbridas y fenómenos cuánticos inducidos por proximidad.*
- *Sensores cuánticos.*
- *Computación cuántica y algoritmos.*

Simposio apoyado por Condensed Matter Physics Center (IFIMAC) y el Departamento de Física de la Materia Condensada de la Universidad Autónoma de Madrid.

List of abstracts at the symposium

Exploring spin at unconventional hybrid interfaces

1st author

Angela Wittmann JGU Mainz

Abstract

Controlled manipulation of a system allows for systematic investigation of the underlying interactions and phenomena. Simultaneously, tunability also enables the development of novel materials systems and devices customized for specific applications. Here, we focus on materials systems that conventionally have not been used as active components in spintronic devices, specifically, hybrid molecule-magnetic interfaces. Molecules offer a unique way of controlling and varying the structure at the interface making it possible to precisely tune the underlying interactions and hybridization at the interface by molecular design. Particularly single-molecule magnets (SMMs) have recently gained significant attention as their multi-level quantum systems promise potential applications in data storage, quantum computing, and spintronics. However, so far, reading and controlling the SMMs has been highly challenging as the functionalization of SMMs on conventional thin-film devices often quenches the quantum character and, thus, the magnetic properties of the molecule due to hybridization effects. Here, we explore the hybridization effects between the SMMs and metal surfaces with the ultimate goal of functionalizing the quantum character in a collective response.

Experimental observation of qubit-magnon interaction

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Abstract

Solid-state quantum computing and quantum sensing technologies rely on the strong coupling between qubits and a quantized field of excitations. Beyond photons, the solid-state offers other bosonic excitations available for emission or absorption, such as magnons, which are the quantum counterparts of spin waves. Magnonic cavities offer the advantage of operating at reduced wavelengths compared to electromagnetic resonators of the same frequency. This is even more appealing with the emergence of magnetic van der Waals materials, which could potentially allow for the implementation of two-dimensional magnonic cavities.

In this study, we explore the spin-magnon coupling between lanthanide molecular qubits and antiferromagnetic spin waves in a van der Waals material. The former comprises a mono-crystal of single-ion magnets consisting of individual gadolinium atoms enclosed within a polyoxometalate moiety. These qubits hold promise for quantum computing applications due to their energy transitions falling within the gigahertz regime and excellent reproducibility. The latter refers to a magnonic cavity embedded within a bulk crystal of CrSBr. This van der Waals offers numerous possibilities for integrating such magnonic cavities into devices. Our experiments unequivocally demonstrate the coupling between spin qubits and antiferromagnetic magnons, representing a crucial step towards achieving substantial qubit-qubit interactions among distant molecular qubits or mediating their interaction with cavity photons for conventional readout protocols.

Dispersive readout of molecular spin qubits

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Abstract

Magnetic molecules are attractive candidates to encode spin qubits [1,2]. We have performed the first experiments to test the dispersive readout of qubits encoded in the spin states of magnetic molecules by means of a superconducting circuit [3]. The molecules are coupled to lumped-element resonators (LERs) fabricated at the Centro de Astrobiología (CAB) [4]. The external magnetic field determines the detuning between the qubit and resonator frequencies. If this detuning is larger than the qubit-resonator coupling, we can perform a non-demolition measurement of the qubit by monitoring the change in the resonator's frequency.

Our sample is PTMr, a free radical with spin 1/2 [5] and the qubit states encoded in its two spin projections. At a given field, the absorption spectrum and longitudinal relaxation time of the radical can be obtained by measuring the shift in the resonator's frequency induced by different driving electromagnetic pulses. The

shape of the shift decay agrees with the distribution of spin-photon couplings generated by a small nano-constriction in the inductor. Finally, the first signs of a coherent manipulation of the spin ensemble have been detected with a specific superconducting chip designed for that purpose.

- [1] A. Gaita-Ariño, F. Luis, S. Hill and E. Coronado, *Nat. Chem.*, 11 (2019) 301-309
- [2] S. Carretta, D. Zueco, A. Chiesa, A. Gomez-Leon and F. Luis, *Appl. Phys. Lett.*, 118 (2021) 240501
- [3] A. Gomez-Leon, F. Luis and D. Zueco, *Phys. Rev. Appl.*, 17 (2022) 064030
- [4] B. Aja, M. C. de Ory, L. de la Fuente, E. Artal, J. P. Pascual, M. T. Magaz, D. Granados and A. Gomez, *IEEE Trans. Microw. Theory Tech.*, 69 (2021) 578-589
- [5] O. Armet, J. Veciana, C. Rovira, J. Riera, J. Castaner, E. Molins, J. Rius, C. Miravittles, S. Olivella and J. Brichfeus, *J. Phys. Chem.*, 91 (1987) 5608-5616

INTW code: Unifying Electron-Phonon Coupling Analyses Across LCAO and Plane-Wave Basis

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Abstract

Over the past decades, first-principles calculations have been crucial in deepening our understanding of many significant problems in physics and materials science. Density Functional Theory (DFT) has played a paramount role in this context, frequently serving as the theoretical foundation for investigating a range of phenomena related to electron-electron or electron-phonon interactions via ab-initio many-body techniques. While there are several available codes for conducting ab-initio many-body calculations, such as Yambo or EPW, which primarily take the output of DFT codes as their input, it's notable that all these options are limited to plane-wave based DFT codes.

In this contribution, we present INTW, a new modular environment to perform many-body calculations from first-principles. The standout feature of INTW, compared to other available tools, is its compatibility with two widely used DFT codes: Quantum Espresso and SIESTA. This offers the significant advantage of allowing users to choose between a plane-wave or an LCAO basis, depending on the specific requirements of the system under study. Additionally, INTW is designed with efficiency in mind, minimizing computational costs by leveraging crystal symmetries to reduce the sampling of the Brillouin zone.

Due to its modular structure, INTW offers a broad spectrum of capabilities for post-processing DFT calculations. Among others, it has been successfully applied to problems requiring the calculation of electron-phonon coupling, Eliashberg function, self-energy functions, and spectral functions [1, 2]. Notably, its application has extended to solving the anisotropic non-linear Eliashberg equations of superconductivity [3] and determining the spin lifetime in magnetic adatoms [4].

- [1] A. Eiguren and C. Ambrosch-Draxl, *Phys. Rev. B* 78, 045124 (2008).
- [2] P. Garcia-Goiricelaya *et al.*, *Comm. Phys.* 2, 81 (2019).
- [3] J. Lafuente-Bartolome *et al.*, *Phys. Rev. B*, 102, 161107(R) (2020).

[4] H. Garai-Marin *et al.*, Phys. Rev. B 107, 144417 (2023).

Tunneling spectroscopy through the magnetic phases of $\text{Ce}(\text{Ru}_{0.92}\text{Rh}_{0.08})_2\text{Si}_2$

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Abstract

The magnetic entropy in a compound containing magnetic ions and itinerant electrons can be reduced to reach the ground state through two competing interactions. Either Kondo screening creates a spin-singlet nonmagnetic coherent state, or Ruderman-Kittel-Kasuya-Yoshida interactions produce magnetic order. CeRu_2Si_2 is an archetypical heavy fermion compound with a large electronic specific heat at low temperatures and no magnetic order. On the contrary, CeRh_2Si_2 presents AFM order below about 36 K. $\text{Ce}(\text{Ru}_{0.92}\text{Rh}_{0.08})_2\text{Si}_2$ shows a combined behavior, with an antiferromagnetic phase (AFM) below 4.2 K, which vanishes above 2.5 T, and a metamagnetic transition at 5.5 T. The electronic properties of $\text{Ce}(\text{Ru}_{0.92}\text{Rh}_{0.08})_2\text{Si}_2$ are highly susceptible to a magnetic field. Here we present atomically resolved tunneling spectroscopy studies in a millikelvin Scanning Tunneling Microscope across the magnetic phase diagram. We visualize directly atomic site dependent Kondo hybridization and its evolution across the different phases with applied magnetic field.

Quantum materials by irradiation of MeV ions

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Abstract

We present our research project on Quantum Materials, based upon exploiting the capabilities of the 5 MV ion-beam accelerator of the tandem type at CMAM to modify various target materials with potential quantum applications.

Specifically, our first focus lies on irradiating diamond crystals, regarded as one of the most promising "quantum materials". Diamond possesses unparalleled physical and chemical properties, rendering it an ideal matrix for high-technology applications. Furthermore, diamond retains much of its quantum features even at room temperature. Our objective is to manipulate the properties of synthetic diamond crystals by irradiating them with either nitrogen (N) or boron (B) MeV ions. In the former case, our aim is to investigate and prepare NV- color centers in diamond in a controlled manner, with the goal of developing quantum sensors capable of measuring the magnetic fields of biological systems. Following irradiation of nitrogen-doped synthetic diamond crystals and subsequent annealing, photoluminescence characterization reveals that we can generate a significant density of NV- centers.

Another ongoing research line is the study of bismuth-antimony alloys, ranging from pure Bi to approximately 20% Sb doping. In their crystalline state, Bi-Sb compounds have been identified as topological insulators. In their amorphous state, they exhibit superconducting properties with critical temperatures around 6 K, making them potential candidates for topological superconductivity. However, Bi-Sb alloys tend to crystallize at higher temperatures, thus presenting a challenge. We are currently exploring various hypotheses and strategies to overcome this issue. Structural, morphological, and electrical characterization of the samples is being conducted, both before and after irradiation with swift heavy ions.

Domain wall networks from intertwined charge density waves in single layer TiSe₂

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Abstract

The commensurate to incommensurate charge density wave (CDW) transition in bulk TiSe₂ remains controversial despite extensive studies. We present atomically resolved STM images of monolayer TiSe₂ revealing an intricate network of CDW domains with significantly larger coherence length than in bulk. Because this system falls in the special category of period doubling CDWs ($Q=G/2$), the order parameter is

real, and the McMillan theory of domain wall formation does not directly apply. We argue that the coupling to a secondary CDW order parameter can explain the presence of domain walls observed in TiSe_2 , different from those predicted by McMillan. We present a Ginzburg-Landau analysis which reproduces the domain wall pattern seen in the experiment.

TaTe₂: A vast landscape of structural and electronic properties.

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Abstract

Transition metal dichalcogenides feature a wide range of physical and electronic properties that range from semiconducting to metallic. Moreover, they can host many-body correlated states such as superconducting phases, Mott insulator phases and charge density waves (CDW) which have brought a lot of excitement to the scientific community.

The most common polymorph of group VI TMDC is the 2H since it is the most stable one. Despite that, other structures can be found in nature, and thanks to the development of new growing techniques, experimentalists can grow large samples of these structures.

Although sulphur and selenium compounds have been thoroughly studied in the past years, tellurium based have been less studied. Interestingly, group V Te-based single-layers are catching attention lately since the absence of Te-Te interlayer interactions changes the electron transfer compared to the bulk or multi-layer cases and new structures and electronic properties can be found [1,2].

In this work [3], we study the structural and electronic properties of single-layer TaTe₂ using first-principles calculations [4]. We find that it presents a large number of possible structures which are very close in energy. We study in detail the formation of these structures and give a possible mechanism for their formation. Moreover, we study their electronic properties in a comprehensive way.

- [1] I. Di Bernardo, et. al. Small 202300262 (2023).
- [2] J. Hwang, et al. Advanced Materials 202204579 (2022).
- [3] J.A. Silva-Guillen, E. Canadell. In preparation (2024).
- [4] A. García. J. Chem. Phys 152, 204108 (2020).

CDW order in the magnetic kagome FeGe

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Abstract

Charge density wave (CDW) ordering is a state, wherein spatial modulation of electronic charge density imposes a new lattice periodicity on a crystal, resulting in the reorganization of electronic bands in the parent phase. The kagome lattice, a geometrically frustrated arrangement of corner-sharing triangles, offers an intriguing platform for exploring intriguing phenomena, including non-trivial band topology, superconductivity, giant anomalous Hall effect or CDW states. Unique electronic characteristics of the kagome net, such as dispersionless flat-bands, van Hove singularities (vHs), and Dirac cones, provide avenues for realizing correlated and topological quantum states.

Recently, a CDW state was discovered in the magnetic kagome compound FeGe, offering insights into the interplay between spin, charge, and lattice degrees of freedom in this type of materials. FeGe demonstrates a sequence of phase transitions, including A-type antiferromagnetic ordering at Néel temperature $T_N = 410$ K, CDW order at $T_{CDW} = 100$ K, and canted magnetic order below $T_{canting} = 60$ K. This underscores the deep intertwining of CDW order with magnetically ordered states, highlighting the role of electron-electron correlations and magnetism. Here, we unveil a charge precursor in FeGe localized at the M point that couples to an order parameter at L due to the geometric frustration of the kagome net, akin to the Ising scenario of antiferromagnetic triangular lattices. We demonstrate the critical role of topological defect unbinding two dimensions to drive the 3D charge order in FeGe.

Investigation on the electronic structure of distorted Kagome magnets RTi_3Bi_4 ($R = Nd, Sm, Gd$)

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Abstract

Kagome materials characterized by geometrical frustration arising from corner sharing triangles have been gathering large attention for their electron correlation, magnetism, topological properties, and the interplay among them [1]. Recently, a new kagome family of AM_3X_4 (A: rare-earth, M: V or Ti, X: Sb or Bi) compounds has been reported, featuring an orthorhombic structure (space group: $Fmmm$) with distorted M kagome lattice [2]. While most of them exhibits low temperature magnetism, the kagome layer remains nonmagnetic, in contrast to the AMn_6Sn_6 family, where strong magnetic interaction exists between A and Mn kagome layers [3]. In addition, the lowered in-plane rotational symmetry would lead to anisotropic kagome bands and topological phases not observed in other kagome compounds. However, experimental investigations on these materials are currently limited. Here, we present the electronic structures of RTi_3Bi_4 ($R = Nd, Sm, Gd$) compounds investigated with angle-resolved photoemission spectroscopy (APRES) and density functional theory (DFT). The anisotropic electronic structure between different M points has been captured, along with band splitting near the Fermi level which might indicate magnetic interactions or surface states. Our findings not only unveil a new kagome family, but also broaden the understanding of quantum phenomena in magnetic kagome materials.

[1] M. Kang *et al.*, *Nat. Commun.* 11, 4004 (2020).

[2] B. R. Ortiz *et al.*, *Chem. Mater.* 35, 9756-9773 (2023).

[3] N. J. Ghimire *et al.*, *Sci. Adv.* 6, eabe2680 (2020).

Softening of a flat phonon mode in the kagome ScV_6Sn_6

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Abstract

Geometrically frustrated kagome lattices are raising as novel platforms to engineer correlated topological electron flat bands that are prominent to electronic instabilities. As well as AV_3Sb_5 ($A = Cs, K, Rb$) and $FeGe$, the kagome system ScV_6Sn_6 hosts a Charge Density Wave (CDW) phase [1,2,3]. Here, we demonstrate a phonon softening at the $k_z = 0.5$ plane in ScV_6Sn_6 at the temperature of the CDW transition phase [4]. Angle-Resolved Photoemission Spectroscopy (ARPES) unveils a momentum-dependent suppression of the intensity due to band folding in the low temperature phase. Inelastic X-Ray Scattering (IXS) and Diffuse Scattering show that the low energy longitudinal phonon collapses at ~ 98 K and $q = (1/3, 1/3, 1/2)$ due to the electron-phonon interaction, without the emergence of long-range charge order which sets in at a different propagation vector $q = (1/3, 1/3, 1/3)$. Theoretical calculations corroborate the experimental finding to indicate that the leading lattice instability is located at $(1/3, 1/3, 1/2)$ of a rather flat mode. We relate the phonon renormalization to the orbital-resolved susceptibility of the trigonal Sn atoms and explain the approximately flat phonon dispersion. Our data report the first example of the collapse of a kagome bosonic mode and promote the 166 kagome compounds as primary candidates to explore correlated flat phonon-topological flat electron physics.

[1] Jiang, YX. et al. Unconventional chiral charge order in kagome superconductor KV_3Sb_5 . *Nat. Mater.* 20, 1353–1357 (2021).

[2] Teng, X. et al. Discovery of charge density wave in a kagome lattice antiferromagnet. *Nature* 609, 490–495 (2022).

[3] Arachchige et al. Charge density wave in kagome lattice intermetallic ScV_6Sn_6 . *Phys. Rev. Lett.* 129, 216402 (2022).

[4] Korshunov, A., Hu, H., Subires, D. et al. Softening of a flat phonon mode in the kagome ScV_6Sn_6 . *Nat Commun* 14, 6646 (2023).

Anharmonic analysis of the possible charge density wave phases on CsV_3Sb_5 using a machine learning interatomic potential

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Abstract

In the recent years a bunch of studies have tried to characterize the emerging CDW phases of the family of kagome topological superconductors AV_3Sb_5 ($A=K, Rb, Cs$). Even though it is known that the phonons in the q -points M and L are responsible for such a transition, the structure of the low-symmetry phase, and the first or second order character of it are still open to debate. In this job, we will take advantage of the Stochastic Self Consistent Harmonic Approximation (SSCHA) to discuss these questions using a machine learning interatomic potential.

The Fermionic-bosonic qubit

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Abstract

We propose a novel superconducting circuit aiming at more robust quantum states, and featuring two distinct quantum degrees of freedom. It consists in the parallel combination of a large inductance, a capacitor and a quasi-ballistic single-channel weak link. The large inductance results in large fluctuations of the phase across the weak link. The weak link implements a Josephson coupling that depends on an internal fermionic degree of freedom associated with the Andreev level. The electromagnetic modes of the circuit depend on the fermionic occupation, leading to a "fermionic-bosonic" qubit.

Joule spectroscopy and heating in hybrid superconductor-semiconductor devices

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Abstract

Hybrid superconductor-semiconductor systems have been widely studied in the past decade for the development of novel quantum devices, with focus on both the topological and trivial regimes. Heat transport, on the other hand, still remains relatively unexplored in such systems, and self-heating effects have been generally overlooked. This is unjustified, considering that heating becomes increasingly more important at very low temperatures, where heat dissipation mechanisms are the least efficient, with potential implications for device performance. To minimize detrimental effects, it is then crucial to understand the fundamental heating and cooling processes in such hybrid systems. In this work, we address these issues by studying devices based on full-shell InAs-Al nanowires. Concretely, we develop a technique dubbed “Joule spectroscopy” that detects Joule effect-driven superconductor-to-normal transitions in a device by means of signatures in electron transport [1]. We further make use of the Little-Parks effect displayed by our nanowires to reveal the dominant heat dissipation mechanism for distinct superconducting regions of a hybrid device. Accordingly, we find that the primary cooling mechanism for grounded and floating superconductors, i.e., quasiparticle diffusion and electron-phonon coupling, respectively, is different. As a result, we conclude that latter is a lot more susceptible to heating, with a cooling power approximately two orders of magnitude lower than grounded superconductors [2].

[1] A. Ibabe, M. Gomez, G. O. Steffensen, T. Kanne, J. Nygard, A. Levy Yeyati, E. J. H. Lee, Nat. Commun. 14, 2873 (2023).

[2] A. Ibabe, G. O. Steffensen, I. Casal, M. Gomez, T. Kanne, J. Nygard, A. Levy Yeyati, E. J. H. Lee, arXiv:2311.13229.

Quantum circuits with multiterminal Josephson-Andreev junctions

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Abstract

In quantum circuits, a conventional tunnel Josephson junction is described in terms of its macroscopic degrees of freedom: the number of tunneled Cooper pairs and its conjugate variable, the phase difference. But this approximation is only valid when the fermionic excitations of the junction itself are far from the lowest circuit levels. In fact, these junctions are just a particular case of a weak link between

superconductors, where their internal structure combines with the superconducting leads to form Andreev bound states, typically examined at a fixed phase difference.

Here [1], we explore the intermediate regime, i.e., a weak link where the phase fluctuations are important, which is now becoming experimentally accessible [2]. We consider a multiterminal junction embedded in different kinds of circuits. On the one hand, we discuss their application to the design of protected qubits by mapping the circuits to the bifluxon and the 0- π qubits [3]. On the other hand, we point out more fundamental questions about their topological properties and their proper quantization rules [4].

[1] Cf. arXiv:2312.17305 (2023)

[2] A. Bargerbos et al., Phys. Rev. Lett., 124, 246802 (2020); M. Coraiola et al., arXiv:2307.06715; T. Vakhtel et al., Phys. Rev. B 107, 195405 (2023), arXiv:2310.03102 (2023)

[3] A. Gyenis et al., PRX Quantum 2, 030101 (2021)

[4] R. P. Riwar et al, Nat. Comm., 7, 11167 (2016), npj Q. Inf. 8, 36 (2022); X. You et al., Phys. Rev. B, 99 174512 (2019)

Characterization of planar Al-based Josephson Junctions proximitized by a ferromagnetic insulator

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Abstract

A ferromagnetic insulator in contact with a superconductor induce an effective exchange field in the latter, emulating the effects of applying an external magnetic field on one superconducting electrode. This, results in a spin splitting of the BCS density of states. In this work, we fabricate and study planar Josephson Junctions made in Ultra High Vacuum conditions using the shadow mask method. These junctions consist of 12,20,30 nm thick aluminum (Al) layers separated by plasma-induced AlOx layers. The ferromagnet used is a 12nm thick of europium sulfide (EuS), a ferromagnetic insulator with a Curie temperature of 16.7K. We characterize the junctions through transport measurements performed at temperatures below 10 mK. We explore the tunnelling current as a function of temperature and magnetic field, observing both quasiparticle and supercurrent components, which attests to the high-quality of the fabricated interface. Our experimental setup provides a means to validate predictions of an enhanced critical Josephson current in junctions featuring spin-split superconductors.

Minimal Kitaev-transmon qubit based on double quantum dots

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Abstract

Minimal Kitaev chains composed of two semiconducting quantum dots coupled via a superconductor have emerged as a promising platform to realize and study Majorana bound states (MBSs), which appear for fine-tuned configurations. We propose a hybrid qubit based on a Josephson junction between two such double quantum dots (DQDs) embedded in a superconducting qubit geometry. The qubit makes use of the 4π -Josephson effect in the Kitaev junction to create a subspace based on the even/odd fermionic parities of the two DQD arrays hosting MBSs. Deep in the transmon regime, we demonstrate that by performing circuit QED spectroscopy on such a hybrid Kitaev-transmon “Kitmon” qubit, one could observe distinct MBS features in perfect agreement with precise analytical predictions in terms of DQD parameters only. This agreement allows us to extract the Majorana polarization in the junction from the microwave response.

InAs-Al nanowire based gatemon qubit

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Abstract

Hybrid superconductor-semiconductor devices are currently under intensive experimental research owing to their rich phenomenology and to their potential in quantum technologies. In particular, these structures are well suited for testing and developing new qubit geometries. In the last decade, there have been several demonstrations of hybrid superconducting qubits based on InAs nanowires with an epitaxially-grown Al layer, including gate-tuneable transmons, also known as “gatemons” [1-4]. Such a qubit architecture presents some interesting advantages when compared to more conventional flux-tuneable transmons, including reduced heating and crosstalk. This has motivated several works to investigate related figures of merit, such as qubit frequency drift [5] or decay and dephasing rates under magnetic fields [6-8]. Still, gatemons constitute a relatively novel and unexplored platform and, therefore, are not fully understood. In this work, I present the latest progress in our efforts to fabricate and study hybrid

superconducting qubits. More concretely, I will show our first cQED measurements of a gatemon qubit fabricated by our group and discuss the gate dependence of its decay and dephasing rates.

1. Larsen, T. W. et al. Phys. Rev. Lett. 115, 127001 (2015).
2. Huo, J. et al. Chinese Phys. Lett. 40, 047302 (2023).
3. Weber, S. J. et al. Nature Nanotechnology 13, 877–878 (2018).
4. Kringhøj, A. et al. Phys. Rev. Lett. 124, 246803 (2020).
5. Casparis, L. et al. Phys. Rev. Lett. 116, 150505 (2016).
6. Sabonis, D. et al. Phys. Rev. Lett. 125, 156804 (2020).
7. Luthi, F. et al. Phys. Rev. Lett. 120, 100502 (2018).

Superconducting devices based on Bi₂Se₃ junctions

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Abstract

Superconductor-based devices have settled the basis for the development of quantum technologies [1], and hybrid devices combining superconductors and topological insulators represent an excellent opportunity for the study of the topological superconducting phase, which offers interesting features that might have significant implications in the development of quantum sensing and quantum computing [2]. On the other hand, the fabrication of new and complex devices can be enriched by the use of focused ion beam techniques, whose versatility enables to create sophisticated devices with high degree of customization [3]. Herein, we develop a novel approach for the fabrication of superconducting devices based on topological-insulator single-crystal Bi₂Se₃ in a geometry characteristic of a superconducting quantum interference device. The characterization of the devices shows that the superconductivity is induced in our crystal and the supercurrent is modulated by the application of an external magnetic field. One of the samples shows an unexpected behaviour with large modulation of the voltage with the magnetic field that cannot be explained with standard models. We propose a scenario in which this behaviour stems from the individual behaviour of one of the Josephson junctions with the interplay of the bulk states present in the crystal and the topological states that appear at the boundary between the crystalline and amorphous phases of Bi₂Se₃ created by the ion irradiation [4, 5].

[1] G. Wendin, Reports on Progress in Physics 80, 106001 (2017)

[2] S. Das Sarma et al., NPJ Quantum Information 1, 15001 (2015)

[3] K. Höflich et al., Applied Physics Reviews 10, 041311 (2023)

[4] A. Bake et al., Nat. Commun. 14, 1693 (2023)

[5] R. Gracia-Abad et al., submitted (2024)

Shaping superconducting proximity effect on graphene with nanometric precision

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Abstract

Graphene can be turned superconducting by the proximity effect. The role of graphene gate-tunable density of states is crucial for understanding the stabilization of a collective proximitized state. Here, we investigate the proximitized superconductivity in graphene bilayers in contact with Pb islands grown on top. In particular, we compare, using LT-STM, the effect of superconducting Pb on graphene grown on the two faces of a polar SiC(1000) crystal. The effect of surface DOS turns out to be crucial. On the Si-side, we identify a collective superconducting state with a small pseudogap, while in the C-side, superconductivity is strong but local. Furthermore, we developed a method to laterally manipulate the Pb islands on graphene and build controllable Superconductor-Graphene structures.

Effects of Coulomb blockade on Josephson phenomena

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Abstract

Effects of Coulomb blockade on Josephson phenomena

The interplay between superconducting correlations and coulomb interaction is important for the proper functionality of superconducting qubits [1]. Disentangling these effects and understanding the consequence of strong Coulomb interactions on superconductivity at the nanoscale is important for superconducting qubits. Here, we study the effects of coulomb correlation on Cooper pair tunneling [2] through a superconducting Pb island on top of graphene. Utilizing a Scanning Tunneling Microscope we measure the spectral properties (Fig 1 (b)) of several island and correlate them with their size (Fig 1 (b)). We approach the problem theoretically with a combination of the PoE and master equation theories [3].

[1] C. Janvier *et. al.*, *Coherent manipulation of Andreev states in superconducting atomic contacts*. Science 349,1199-1202(2015). DOI:10.1126/science.aab2179

[2] P. Joyez. *The single Cooper pair transistor: a macroscopic quantum system*. Superconductivity [cond-mat.supr-con]. Université Pierre et Marie Curie - Paris VI, 1995. English. ?NNT : ?. ?tel-00534358?.

[3] G. L. Ingold and Yu. V. Nazarov, in *Single Charge Tunneling: Coulomb Blockade Phenomena in Nanostructures*, edited by H. Grabert and M. H. Devoret (Springer US, Boston, MA, 1992) pp. 21–107

Optical probes for the unconventional normal state of twisted bilayer graphene

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Abstract

Twisted bilayer graphene (TBG) and other moiré systems are ideal platforms to explore different phases which may be exploited in devices for future quantum technologies. In order to fully understand the various phenomena observed in these materials, it is crucial to characterise their normal state from which different phases (superconducting, insulating, magnetic or intervalley coherent) arise. In particular, even at temperatures above which the ordered phases occur, spectroscopic measurements [1] and compressibility [2] show electronic resets as a function of filling in the form of cascades. We have recently shown [3] that the observed cascades are associated to the formation of local moments and heavy quasiparticles and not to symmetry broken orders, which occur at lower temperatures. Our results, which account for the dynamical correlations, are based on Dynamical Mean Field Theory plus Hartree calculations. We reproduce the cascade flow of spectral weight, the oscillations of the remote band energies, the asymmetric jumps of the inverse compressibility, the presence of resistive states at integer fillings, and predict a strong momentum differentiation in the incoherent spectral weight associated to the fragile topology of TBG [3]. The strong correlations behind this complex phenomenology may also impact other measurements that can be used to characterise the normal state. In particular, optical probes, which connect states with the same momentum spin and valley, may reveal complementary information about the nature of the electronic states involved at different frequencies. In this talk I will introduce the properties of the peculiar normal state of TBG and will show how the cascades manifest in the optical spectrum.

[1] D. Wong et al, Nature 582, 198 (2020); Y. Choi et al, Nature 589, 536 (2021).

[2] U. Zondiner et al, Nature 582, 203 (2020).

[3] A. Datta, A. Camjayi, M.J. Calderón and E. Bascones, Nature Comm. 14, 5036 (2023)

Disorder reduces localization in magic-angle twisted bilayer graphene [1]

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Abstract

Flat bands in Moiré systems, and their localization in real space, have been connected with exotic correlated physics, such as the superconducting and Mott insulating phases of Magic-Angle Twisted Bilayer Graphene (MATBLG) [2-4]. This happens because the vanishing kinetic energy and the real-space localization trigger a dominant Coulomb interaction. The role of the Moiré superlattice potential in this phenomenon is well known, but the roles of structural (twist-angle) and electrostatic disorder remain unclear.

In this presentation we will discuss what is known about the effect of disorder on MATBLG, and present simulation results showing that the inclusion of electrostatic disorder in MATBLG can lead to delocalization in the flat bands, increasing the electronic mean free path [1]. This suggests that even weak disorder can have a strong impact on the Coulomb interactions that drive the exotic physics of these systems.

1. PA Guerrero, VH Nguyen, AW Cummings, JH García, JC Charlier, S Roche, arXiv:2401.08265
2. Y Cao, V Fatemi, S Fang, K Watanabe, T Taniguchi, E Kaxiras, PJ Herrero, Nature, 566 (2018) 43
3. P Stepanov et al, Nature, 583 (2020) 375
4. R Bistritzer and AH McDonald, PNAS, 108 (2011) 12233

Anharmonic effects clarify the mechanical and acoustic properties of graphene

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Abstract

Despite many of the applications of graphene rely on its uneven stiffness and high thermal conductivity, understanding its mechanical and acoustic properties, as well as those of 2D materials in general, remains challenging. Harmonic theory predicts a quadratic dispersion for the out-of-plane flexural acoustic vibrational mode, which leads to the unphysical result that long wavelength in-plane acoustic modes decay before vibrating one period, preventing the propagation of sound. The robustness of the quadratic dispersion has been questioned by arguing that the anharmonic phonon-phonon coupling between in-plane and out-of-plane phonon modes linearizes it, which implies a divergent bending rigidity in the long wavelength limit not reproduced experimentally. By including anharmonicity in a non-perturbative way within the Stochastic Self-Consistent Harmonic Approximation (SSCHA), we show that rotational symmetry protects the quadratic flexural dispersion against phonon-phonon interactions, ensuring that the bending stiffness remains non-divergent regardless of temperature. Our non-perturbative anharmonic calculations demonstrate that sound propagation indeed coexists with the quadratic dispersion. We also show that the temperature dependence of the height fluctuations of the membrane, known as ripples, is fully determined by thermal or quantum fluctuations, but without the previously assumed anharmonic suppression of their amplitude. These conclusions should hold for all strictly two-dimensional materials.

Noise correlation measurements: a new approach to detect spontaneously symmetry-broken phases with ultracold atoms

1st author

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Abstract

Spontaneously symmetry-broken (SSB) phases are locally ordered states of matter characterizing a large variety of physical systems. Because of their specific ordering, their presence is usually witnessed by means of local order parameters. Here, we propose an alternative approach based on statistical correlations of noise after the ballistic expansion of an atomic cloud. We indeed demonstrate that probing such noise correlators allows one to discriminate among different SSB phases characterized by spin-charge separation. As a particular example, we test our prediction on a 1D extended Fermi-Hubbard model, where the competition between local and nonlocal couplings gives rise to three different SSB phases: a charge density wave, a bond-ordering wave, and an antiferromagnet. Our numerical analysis shows that this approach can accurately capture the presence of these different SSB phases, thus representing an alternative and powerful strategy to characterize strongly interacting quantum matter.

Quantum Many-Body phase diagram characterization using Fidelity-based Kernels

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Abstract

The use of fidelities in Quantum Theory has a long history that has enhanced our understanding of quantum systems. In Quantum Many-body physics, detecting Quantum Phase Transitions (QTPs) without conventional order parameters is of particular interest, as these parameters may not work for some models. In such cases, Quantum Machine Learning (QML) comes into play, along with quantum fidelities. Our study of QTPs utilizes physics-inspired Quantum Kernels tailored to celebrated fidelities such as the Uhlmann and the Susceptibility fidelity. We leverage these Quantum Kernels for Anomaly Detection in an unsupervised setting - the anomalies being the quantum phase transition boundaries. In the Figure, we efficiently recognize the different phases of the Axial Next-Nearest-Neighbour Interaction (ANNNI) model already for spin chains of small sizes supporting the validity of our QML model.

Physically motivated enhancements of variational quantum eigensolvers for quantum chemistry

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Abstract

The Adaptive Derivative-Assembled Pseudo-Trotter Variational Quantum Eigensolver (ADAPT-VQE) has emerged as a promising approach in quantum chemistry. Nevertheless, the application of ADAPT-VQE with noisy quantum devices requires to enhance its efficacy. Leveraging insights from electronic structure

theory, we concentrate on optimizing state preparation without added computational burden and guiding ansatz expansion to yield more concise wavefunctions with expedited convergence toward exact solutions. These advancements culminate in shallower circuits and reduced number of measurements. The performance of the new ADAPT-VQE variants will be assessed across mono, di, and tridimensional arrangements of H4 models, as well as in the ground state calculation of the water molecule. Ultimately, this work attests to the viability of physically-motivated strategies in fortifying ADAPT-VQE's efficiency, marking a significant stride in quantum chemistry simulations.

Projected Lindbladian Dynamics via Hamiltonian Symmetries for Quantum Error Mitigation

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Abstract

Quantum error mitigation (QEM) techniques have shown extremely good promise for computing in the NISQ-era. Some widely-accepted QEM methods have converged into to the so-called Probabilistic Error Amplification (PEA) based zero-noise extrapolation (ZNE). This method assumes that the ideal (target) expectation value of operators are functions of noisy values of those measured at different noise rates. Moreover, it is not generally easy to make assumptions of the decay tendencies of the observables, specially when non-Clifford circuits are targeted. Some methods attempt to learn those by substituting most of the gates of a circuit by Clifford gates (Clifford Data Regression, CDR) or by small-scale tractable circuits. However, changing the circuit changes the noise and, thus, what is learnt might not be always accurate for the target circuit. In this work, we propose a method based on projecting the ideal expectation values onto a linear span of noisy measurements. In order to train the coefficients for the linear span, we make use of observables whose expectation values are conserved over the dynamics (Hamiltonian symmetries). Specifically, we probe the noisy processor to obtain noisy expectation values (at different noise rates) of quantities that are conserved and, therefore, known, for obtaining the projection weights. The obtained model is then used to mitigate the noise of the target observables of interest. In this way, the circuits for which the training is made are exactly the same as for the actual experiment. We numerically analyse the proposed method for studying the magnetization in the transverse field Ising and Heisenberg models. We will also discuss the potential of the method for discerning which is the function that defines the decays of the observable. We will also present the future research on the topic.

Coherent nuclear spin dynamics in graphene-related carbon nanostructures

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Abstract

Based on a numerical method to obtain hyperfine tensors for planar π -magnetic sp^2 hydrocarbons, we explore the coherent hyperfine physics engendered by these interactions and explore their implications for electron and nuclear spin qubits in these structures. We discuss quantitatively the electron-spin decoherence beyond the quasistatic approximation and show how to optimize it for a given molecule. We then determine the effective nuclear spin Hamiltonian mediated by the electron spin and investigate its consequences for the storage and manipulation of nuclear spin qubits.

Localisation, Thermalisation and Time Crystals: Quantum Simulations of Disorder

1st author

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Abstract

Dynamical quantum systems provide a rich playground to study a number of fundamental questions in quantum mechanics regarding localisation, ergodicity and entanglement growth. Classical methods such as tensor networks can be used to study these phenomena but are restricted to certain paradigms such as short-time simulations or systems with weak entanglement growth. It is thus not always clear from numerical simulations whether an observed physical phenomenon is an artefact of the structure imposed on the Hilbert space by the tensor network algorithm or is indeed a true reflection of a quantum mechanical system. In this work, we use a quantum computer to address this issue. We consider a Hamiltonian with disordered couplings and implement its dynamics on a quantum computer. We ask the following questions: can we observe a low dimensional discrete time crystal in an *interacting* system on a real quantum device? Can we observe the localisation/thermalisation transition on a quantum computer? If the ergodic regime is difficult to study with classical numerics, can the quantum computer provide more accurate results?

Quantum computation of the dynamics of a quantum emitter coupled to an optical nanoresonator

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Abstract

The interaction between excitons in quantum emitters and optical resonators is key for a variety of applications ranging from improved molecular sensing to the design of faster photon sources. Further, when the coupling strength overcomes the losses of the system, the strong coupling regime is reached, where the response of the system is governed by hybrid excitations with novel properties. We first describe how plasmonic resonances excited in metallic nanostructures are very attractive in this context, because

they allow for maximizing the coupling strength by confining the optical field well below the diffraction limit. As a consequence, the strong coupling with single quantum emitters can be achieved also at room temperature, where strong losses are unavoidable. We present recent results that have pushed light confinement to its ultimate limits by exploiting subnanometer gaps and atomic-sized protrusions. We then obtain the response of these systems using an IBM quantum computer. We focus on a simple canonical situation where a quantum emitter, which is treated as a two-level system, couples strongly with a single plasmonic mode. The interaction is described with the Jaynes-Cummings Hamiltonian. To compute the Rabi oscillations that characterize the dynamics of this system, we first implement the qubitization of the bosonic plasmonic mode [1,2]. We find that, surprisingly, the trotterization error can be zero under certain conditions when using an appropriate qubitization and a specific grouping of the different terms of the Hamiltonian. Thus, this work contributes to the understanding of the promise of quantum computing for nanophotonics. Notably, the generalization of the Jaynes-Hamiltonians can become very computationally demanding for classical algorithms, for example if many quantum emitters are included to engineer new sources of quantum light.

[1] R. D. Somma arXiv: quant-ph/0512209 (2005).

[2] Xin-Yu Huang et al., arXiv:2105.12563, 2021

Manipulation of hole spins under realistic electric and strain fields in quantum dots

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Abstract

In recent years, there has been a growing interest in utilizing hole spins in silicon and germanium for quantum information processing. One reason for this is the strong spin-orbit interaction present in the valence band of these materials, which allows for versatile interactions with electric fields. As a result, there have been demonstrations of fast electrical manipulation of hole spin qubits [1] and strong spin-photon interactions [2], which are useful for generating long-range entanglement, all mediated by spin-orbit interactions. Interestingly, recent experiments in Ge hole qubits have shown efficient manipulation with in-plane magnetic fields [3], which cannot be easily explained by the expected spin-orbit mechanisms, such as cubic Rashba or g-tensor modulation resonance.

In this work, we go beyond the usual models for electrical spin manipulation in semiconductor quantum dots. We perform simulations of realistic Ge devices and find that both the electrostatics [4] and the strain [5] display inhomogeneities that dominates the performance of hole spin qubits. In particular, we identify overlooked spin-orbit mechanisms mediated by strains and the interfaces [6] that enable manipulation under in-plane magnetic fields and enhance the expected Rabi frequencies. Our simulations show that these mechanisms are dominating the physics of isotropic hole spin qubits.

[1] G. Scappucci et al., Nat. Rev. Mater 6, 926-943 (2021)

[2] C. Yu et al., Nat. Nano. 18, 741–746 (2023)

[3] N. Hendrickx et al., Nature 591, 580–585 (2021)

[4] B. Martínez et al., Phys. Rev. B 106, 235426 (2022)

[5] J. C. Abadillo-Uriel et al., Phys. Rev. Lett. 131, 097002 (2023)

[6] E. Rodríguez-Mena et al., Phys. Rev. B 108, 205416 (2023).

Superconductivity at low pressure conditions in Rb – H system

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Abstract

The highest measured superconducting critical temperature was achieved in the high-pressure hydrides[1]. However, the high pressures needed to stabilize these structures preclude their technological application. Thus the focus of the field shifted to finding polyhydride materials that are stabilized at lower pressures. Here we are reporting a possibility of high-temperature superconductivity in rubidium hydrides at low pressures. We find that RbH₁₂ in the hexagonal phase can be stabilized at pressures below 5 GPa and shows critical temperatures comparable to the best conventional superconductors. Although at 5 GPa RbH₁₂ is above the convex hull, we show that at 50 GPa and including the quantum and anharmonic effects [2] the probability of synthesizing these materials increases. Furthermore, we calculate several structural and spectrographic signatures of these structures to aid in their identification during synthesis. The estimated superconducting critical temperature increases with pressure and reaches liquid nitrogen temperatures at 25 GPa.

[1] Chris J Pickard, Ion Errea, Mikhail I Erements, *Annu. Rev. Condens. Matter Phys.* 2020. 11:57–76.

[2] Lorenzo Monacelli, Raffaello Bianco, Marco Cherubini, Matteo Calandra, Ion Errea, Francesco Mauri, *J. Phys.: Condens. Matter* 33 363001 (2021).

Detection system and oscillation decay of a superconducting sphere immersed in superfluid ⁴He.

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Abstract

Detection system and oscillation decay of a superconducting sphere immersed in superfluid ⁴He.

We report here the experimental progress of our apparatus for the study of superfluidity using magnetic levitation [1]. The design consists of a set of coils that allow levitating a superconducting sphere of type I superconductor immersed in a superfluid.

First, we have developed a system capable of detecting the position of the sphere without the use of high energy radiations that could destroy the superfluidity in future experiments in He³. This system is based on the change in inductance that a coil undergoes when moving a diamagnetic object in its vicinity [2].

We have also performed several levitation experiments using a He⁴ optical cryostat trying to emulate the experiments performed by Schoepe et al. [3], where we have measured the decay of the oscillations for different temperatures, both in laminar and turbulent regime.

[1] M. Arrayás J.L. Trueba C. Uriarte D. Zmeev, *Scientific Reports* 11, (2021).

[2] M. Arrayás et al. *J. Low Temp. Phys.* 212 (2023) .

[3] R. Hanninen and W.Schoepe, J. LowTemp.Phys. 11, (2010).

Quantum geometry and disorder

1st author

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Abstract

During the last decades, the Berry curvature has been the cornerstone of topological matter. But recently, it has been shown that it is only one of the two faces, the imaginary one, of a more general structure called the Quantum Geometric Tensor. The other size, the real part, usually called the quantum metric, has been receiving a lot of attention lately as it has been shown to play a crucial role in the superconductivity of flat bands materials, linear and non-linear response theory and a large compendium of other effects. Moreover, it has been proven that the quantum metric is a key quantity in the Modern Theory of insulators, as it is directly related to the real-space localization of the ground state. In this work we make two huge developments on this new quantity: first, we show a numerically efficient way of computing it via linear-size scaling algorithmics based on the Kernel polynomial method that allows us to study huge inhomogeneous systems and secondly, using this method, we have studied the Quantum metric in the presence of disorder showing its properties in more realistic conditions.

Anisotropic superconductivity with few Helmholtz Fermi-surface harmonics

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Abstract

We present an efficient method to compute the critical temperature, superconducting gap and related physical properties of anisotropic superconductors from first principles, which yields an efficiency gain of several orders of magnitude with respect to the state-of-the-art techniques. Our method is based on a linear transformation from momentum space to a set of orthonormal functions defined as the solutions of the Helmholtz equation on the Fermi surface. In this way, all the anisotropy of the problem is described by a handful of coefficients with built-in symmetry. As a proof-of-principle, we apply our method to solve the anisotropic Eliashberg equations in conventional phonon-mediated superconductors, for which the electron-phonon coupling matrix elements are computed from first principles with the INTW code. The simplification introduced by our method enables the high-throughput exploration of superconducting

materials, and opens up new avenues for the development of ab initio approaches to more advanced theories of superconductivity.

POSTER: On-surface synthesis of nanographenes on proximitized superconducting substrates.

Presenter

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Abstract

Bridging magnetism and superconductivity has always been a fascinating field where many rich physical phenomena emerge. Exploring molecular magnetism on superconducting substrates has the advantage over atomic spins of selectively tuning the exchange interaction with the underlying substrate through molecular structural design. However, most elemental superconductors have highly reactive surfaces which result in the decomposition of the molecular species upon adsorption. To tackle this problem, we fabricated a metallic proximitized superconducting platform to achieve on-surface synthesis of molecular nanostructures while maintaining the superconducting properties of the substrate. First, we explore the growth of Ag on a Nb(110) single crystal, where we find 10-30nm-high superconducting Ag(111) islands [1] grown on top of an Ag/Nb wetting layer. The Ag islands not only manifest the proximitized superconducting gap but also several in-gap states of non-magnetic origin [2,3]. On this substrate, we deposited two types of fully organic molecules hosting open-shell magnetism, to study the interaction of the pi-molecular spins with both regions of the substrate, the Ag/Nb wetting layer and the bulk Ag islands. On triangulene chains, which on a Au(111) pristine surface build up a $S=1$ Haldane chain with fractional spin end states [4], we find a clear magnetic fingerprint, manifested as in-gap Yu-Shiba-Rusinov (YSR) states, over some unities of the chain. These were attributed to the interaction of intrinsic defects in the chains because regularly formed chains show no magnetic signal. Similarly, no magnetic signal was found for the 2OS diradicals probably due to the distinct geometry of the molecule resulting in a closed-shell structure, contrary to the case of Au(111) [5]. Our results pave the way towards the combination of superconductivity and molecular magnetism at the atomic level.

[1]: Tomanic, Tihomir, et al., Physical Review B 94(22), 220503 (2016).

[2]: Machida, K. & Shibata, F. Prog. Theor. Phys. 47, 1817–1823 (1972).

[3]: Schneider, L., Ton, K.T., Ioannidis, I. et al. Nature 621, 60–65 (2023).

[4]: Mishra, S., Catarina, G., Wu, F. et al., Nature 598, 287–292 (2021).

[5]: A. Vegliante et al, arXiv:2402.08641 (2024)

POSTER: Phase Analysis in FeSe

Presenter

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Abstract

FeSe is one of the simplest iron-based superconductors, despite not being magnetic itself. Exhibits both nematicity and superconductivity, which are highly tunable. Its superconductivity is based in an orbital selective pairing mechanism and its Fermi surface shows three bands with different orbital characters. FeSe has a critical temperature of 8 K but can be risen to 37 K under pressure or 65 K as monolayers deposited on SrTiO₃.

We report on the observation of the vortex lattice, between 10 T and 14 T. We also observe magnetic field dependent charge order, providing new relevant information about the hypothesized new high field modulated superconducting phase [Phys. Rev. Lett. 127, 257001 (2021)].

POSTER: Design of 2D Rare Earth – Au substrates for Spin Studies on Magnetic Nanographenes

Presenter

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Abstract

The synthesis of monolayer rare earth – gold intermetallic compounds with high crystallinity on a Au(111) surface opened the doors to a new set of magnetic surfaces for the on-surface synthesis of graphene nanostructures [1,2]. All these reported rare earth – noble metal compounds show a hexagonal moiré pattern and a RE-NB₂ stoichiometry. There are two key aspects of these REAu₂ monolayers: their ferromagnetic character [3] and their reduced work function with respect to Au(111) [1]. In this work, we benefit from these two properties to perform SPM techniques to further explore the spin properties of triangulene nanostructures.

Here we study first the on-surface synthesis of [3]-triangulene (3T) chains on GdAu₂ and on HoAu₂. The first substrate shows antiferromagnetically aligned domains in spin polarized STM images. Here, we detected spin-asymmetry maps of the semi occupied orbital of the AFM 3T chains. However, the strong magnetic coupling with the surface hinders the observation of inelastic spin-excitation features related to the presence of radical electrons at the termini [4]. On the other hand, HoAu₂ doesn't show antiferromagnetic domains in SP-STM, but spin excitation spectroscopic features remained, probably caused by a smaller coupling with the chains.

We also explored the on-surface synthesis of aza-[3]-triangulene (A3T) on GdAu₂. A3T tends to donate charge on a Au(111) surface [5]. By measurements of local contact potential difference (LCPD) using Kelvin probe force microscopy (KPFM) we show that A3T remains more positively charged on Au than on GdAu₂, reaching in this case a mix valence regime. These experiments serve as proof of concept of the suitability of these surfaces to perform advanced SPM techniques that are not possible on Au(111) to deepen our knowledge about spin states in nanographenes.

[1] Y. Que et al. *J. Phys. Chem. Lett.* 11, 5044-5050 (2020)

[2] J. Brede et al. *Nat. Commun.* 14, 6677 (2023)

[3] L. Fernández et al. *Nanoscale* 12, 22258 (2020)

- [4] S. Mishra et al. *Nature* 598, 287-292 (2021)
[5] T. Wang et al. *J. Am. Chem. Soc.* 144, 4522-4529 (2022)

POSTER: Electronic friction between two graphene sheets

Presenter

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Abstract

Most of tribology responds to adiabatic processes in which phonons and/or structural deformation and chemical reactions give rise to energy dissipation. Recently, however, electronic friction has been observed in some energy-dissipation processes, like in nanoscale water flows in carbon nanotubes. Beyond a landmark theoretical paper including electronic friction in linear response, the literature on the subject is quite limited. In this work, we study electronic effects in a system consisting of two graphene layers at graphitic distance moving parallel to each other. We study its dependence on interlayer distance and the mutual velocity of the layers. Results will be shown for real-time time-dependent density functional theory (TD-DFT) as implemented in the SIESTA code, complemented by some theoretical limiting values.

POSTER: Atomic Force, Kelvin Probe and Scanning Tunneling Microscopy of graphene and twisted graphene

Presenter

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Abstract

Atomic Force, Kelvin Probe and Scanning Tunneling Microscopy of graphene and twisted graphene

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We have explored the response of the 2D electrons in graphene and two-dimensional materials by means of Scanning Tunneling Microscopy (STM), Atomic Force and Kelvin Probe Microscopy (AFM, KPFM). STM and KPFMs spectroscopy allow to study how the interplay between local atomic structure, topology, and electrons' correlation, which determines the electrons behavior [1,2]. We have studied graphene and twisted graphene on hBN, imaging the structure, topology, and electronic properties of the materials.

[1] J. Yu et al, "Imaging Graphene Moiré Superlattices via Scanning Kelvin Probe Microscopy", Nano Lett. 7, 3280 (2021).

[2] C. Zhang, T. Zhu, T. Soejima, S. Kahn, K. Watanabe, T. Taniguchi, A. Zettl, F. Wang, M. P Zaletel, and M. F. Crommie "Local spectroscopy of a gate-switchable moiré quantum anomalous Hall insulator", Nat. Commun. 14, 3595 (2023)

POSTER: Excitonic insulators in monolayer transition metal dichalcogenides

Presenter

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Abstract

Under certain circumstances in terms of the electronic structure and the Coulomb interaction strength, a bandgap can be opened in the band structure of a material due to the condensation of electron-hole pairs, that is, an excitonic condensate. Even though it had been proposed in the past, it has not been until the recent years that experimental evidence may support the existence of this state in transition metal dichalcogenides monolayers.

In particular, monolayer 1T' WTe₂ has shown a plethora of promising correlated quantum states, from quantum spin hall insulating to unconventional superconducting phases. Without interactions, monolayer 1T' WTe₂ is semimetallic, therefore electron and hole Coulomb instabilities could drive the pairing mechanism for the observed experimental behaviors. Moreover, a repulsive on-site interaction mechanism has been proposed theoretically as the origin of unconventional superconductivity that appears at low-density electron doping.

In this work, we employ a Hartree-Fock approach to characterize the excitonic states that arise in the system and we construct the correlated phase diagram of this material. We find two different excitonic domes and analyze their particular spin ordering. Interestingly, each dome features a different ground state, one with a spin density wave (SDW) and the other with a spin spiral (SS) state. This SS is compatible with the lack of charge modulation observed in the experimental data.

POSTER: Tuning NbTiN superconducting resonators for quantum computing applications

Presenter

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Abstract

Superconducting resonators play a crucial role in many trending technological areas such as quantum computing, quantum sensing, and astronomy. Among the different types of resonators, Lumped Element Resonators (LERs) show appealing properties such as their small size compared to their wavelength, the frequency multiplexing that allows reading them out with a single transmission line, and the control over their field mode volume. Moreover, the superconductor nature of these resonators offers several advantages, including a very high sensitivity and extremely low losses.

Another relevant advantage for many applications is the contribution of the kinetic inductance (L_k) to their resonant frequency (f_{res}), which has a nonlinear behavior. This kinetic inductance can be controlled through either a DC current flowing through the inductor or by an RF pulse generated near the resonance frequency. To maximize the range over which f_{res} can be tuned, it is important to maximize its dependence on L_k . This can be done in different ways: reducing the thickness of the superconducting film or choosing a material with an intrinsically high L_k . In this regard, NbTiN offers a higher L_k than other traditionally used materials such as Al or Nb.

The recent introduction of superconducting resonators as a suitable basis to operate spin-based quantum processors offers a perfect opportunity to exploit this tunability. Of particular interest are platforms based on electronuclear spin qubits, which allow embedding non-trivial operations, even quantum error correction, and those involving spins with avoided level crossings (spin clock transitions) that mitigate the decoherence induced by magnetic noise sources. Yet, they also call for ways to operate with multiple transitions whose characteristic frequencies depend weakly on the magnetic field. Here, we present our recent progress in the development and optimization of NbTiN tunable resonators for quantum applications, where the two different tuning methods are successfully tested at low temperatures.

POSTER: Phonon Topology in AgP2

Presenter

Francisco Manuel Ballester Macià DIPC - Donostia International Physics Center

Co-presenters

Ion Errea Lope University of the Basque Country CFM - Centro Física de Materiales

Maia García Vergniory Max Planck Institute for Chemical Physics of Solids DIPC - Donostia International Physics Center

Abstract

Due to recent developments in Topological Quantum Chemistry, the study of the topological properties of electronic systems is well known. However, for phononic systems the implications of topological labels are not fully understood. Using the tools developed for the creation of the Topological Phonon Database, we will study the case of AgP2 (mp-ID: mp-8200): an ideal case of an Obstructed Atomic Band Representation (OABR). More precisely, we will obtain the surface states of AgP2 and see how they are influenced by the bands corresponding to OABRs. Afterwards, we will show the effect of topology on the selection rules for Raman and IR scattering of this compound.

POSTER: Phononic Casimir effect

Presenter

Pablo Rodriguez Lopez Universidad Rey Juan Carlos and GISC

Co-presenters

Dai-Nam Le University of South Florida

Lilia M. Woods University of South Florida

Abstract

Fluctuation-induced interactions are a universal effect that need a fluctuating field and the induction of noise to generate a macroscopic transport of energy (heat transfer) or momentum (Casimir effect) between macroscopic objects. Here we present the phononic Casimir effect, a fluctuation-induced interaction mediated by phonons instead of the usual electromagnetic field. We will show, on one hand, how to couple the phononic modes of separated compact objects that opens a new channel for heat transfer and Casimir effect in the very close regime, and on the other, how the coupling with the electromagnetic field will modify the em Casimir effect, leading even to an unusual repulsive Casimir effect for a kind of piezoelectric materials. Those results pave the way for an understanding of the forces on a superconducting sphere immersed on a superfluid, an experiment that is being carried out by our group, where we expect that the phononic modes will be one of the relevant contributions on the forces over the sphere.

Energy transition: materials, technologies and sustainability (DFMC-GEFES, GEE) / *Transición energética: materiales, tecnologías y sostenibilidad (DFMC-GEFES, GEE)*

Organiser

Pablo Palacios(UPM) Celia Polop (UAM) Ferry Prins (UAM)

Invited speakers

Georgia T. Papadakis (ICFO) Miguel Angel Niño Ortí (ALBA) Miguel Anaya (US) Leire Zubizarreta (ITE)

Symposium abstract

The transition to a carbon-neutral society relies in large part on the development of materials and technologies for improved energy harvesting, conversion, and storage. This is a joint symposium between GEE and GEFES in which we will discuss the latest advances in materials and technologies for solar cells, battery storage, and green hydrogen production. In particular, we will highlight the underlying physics that governs their functioning and the structure-property relationships that can be leveraged to rationally design the next generation of energy technologies. Ranging from material preparation to characterization, from device modelling to their operation and passing through efficiency and sustainability issues, this symposium aims to forge collaborations to accelerate the deployment of materials that will power the energy transition and shape a greener future.

La transición hacia una sociedad neutra en carbono depende en gran medida del desarrollo de materiales para mejorar la recolección, conversión y almacenamiento de energía. En este simposio, discutiremos los últimos avances en materiales para células solares, almacenamiento de baterías y producción de hidrógeno verde. En particular, destacaremos la física subyacente que gobierna su funcionamiento y las relaciones estructura-propiedad que pueden aprovecharse para diseñar racionalmente la próxima generación de tecnologías energéticas. Este simposio, que abarca desde la preparación de materiales hasta la caracterización y desde el modelado de dispositivos hasta su funcionamiento, tiene como objetivo forjar colaboraciones para acelerar el despliegue de materiales que impulsarán la transición energética y darán forma a un futuro más ecológico.

List of abstracts at the symposium

The nanoscale landscape dictates performance in perovskite solar cells

1st author

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Abstract

Halide perovskites are generating enormous excitement for their use in high-performance yet inexpensive optoelectronic applications. Nevertheless, these solution processed materials have a plethora of micro- and nano-scale heterogeneities and their impact on performance and stability need to be understood. In this presentation, I will discuss our work to determine the relationship between material structure, chemistry and photophysical properties on the nanoscale using advanced microscopy techniques. I will show how synchrotron nanoprobe and optical spectroscopic methods correlated at the nanoscale explain why halide perovskites are remarkably tolerant to defects. These observations reflect that the quest of highly pristineness in traditional semiconductors is not necessarily a condition for low temperature, solution processed halide perovskites to perform well when integrated into devices. Further, I will discuss how measuring photoluminescence as a function of voltage allows us to extract pseudo-JV curves and device performance metrics with sub-micron spatial resolution. Spatially correlating these measurements with synchrotron nanoprobe X-ray fluorescence, we decouple how different device architectures influence

nanoscale degradation. We will comment on the implications these findings have for microscopically improving device stability.

Oxygen evolution reaction: the bottleneck in the production of electrocatalytic green hydrogen revealed by operando X-ray spectroscopy

1st author

Juan Jesús Velasco Vélez ALBA synchrotron

Abstract

Water splitting is accounted as one of the most important electrochemical processes for the storage of renewable energy by the cathodic production of molecular hydrogen that can be used as a carbon-free energy vector. However, the sluggish anodic oxygen evolution reaction (OER) limits significantly the efficiency of this technology and as a consequence its economic viability. Moreover, the electrode corrosion under acidic conditions and anodic polarization shortens materials lifetime with the consequence of the increase of the costs. Among all the materials investigated for the OER, iridium and its oxides/hydroxides combine uniquely the lowest overpotential and highest corrosion resistance under harsh acidic conditions. Unfortunately, iridium is also one of the rarest and scarcest elements on earth, thus synthetic strategies for its optimal usage are required. We reason that determining the electronic structure characteristics responsible for the peculiar reactivity of IrOx during OER is key to extend these unique properties to a more abundant material. Unfortunately, the element specific analytical techniques able to provide interface information are very limited and hardly compatible with liquids allowing usually only ex situ characterizations methods. This limitation led to a loss of important information as in many cases the reaction intermediates and electrocatalytic active species cannot be “quenched” in post process analysis. Herein, we combine surface and bulk sensitive X-ray spectroscopy techniques together with the precise nano-fabrication of nanostructure thin films to determine the nature of the active species and their distribution in the surface and near-surface region during the electro-catalytic process yielding a clear description of the species ruling the stability and activity of IrOx during OER conditions.

Hysteretic adsorption of Molecular Hydrogen in Double Wall Carbon Nanotubes bundles

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Abstract

Carbon nanostructured materials are regarded to have high potential for the storage and management of H₂ at cryogenic temperatures. We have observed isothermal large hysteretic hydrogen adsorption in samples made out of Double Wall Carbon Nanotubes bundles at 50 K, 77 K and 150 K and up to 15 bar of pressure [1]. Adsorption metastability opens remarkable possibilities: it can be used to lower the working pressure for a given uptake; to increase the usable capacity; or to facilitate thermal management. Metastable H₂ adsorption, however, has been barely explored, mostly in the context of Metal-Organic Frameworks (MOFs) [2]. For nanostructured carbons, hysteresis has been associated with chemisorption in

metallic particles [3], characterized by undesirably high desorption energy barriers. To gain physical insight, we made a series of inelastic neutron scattering measurements. The elastic signals at different H₂ loads are consistent with the uptake of the H₂ within the interstitials of the bundles. The quasielastic signal display an anomalous dependence on momentum transfer which is nicely reproduced by an accurate 1D dimensional diffusion model (as expected from interstitial confinement of the H₂ fluid) while the complete inelastic signal precludes the possibility of chemisorption onto the sample metallic impurities. We have developed a two-dimensional model that reproduces the qualitative behaviour of the real system. It sheds light in the microscopic mechanisms responsible of the observed metastability, in particular, in the role played by the hierarchical structure of energy and entropic barriers emerged as a consequence to the two-dimensional configuration of the bundle interstitials.

1. C. Cabrillo *et al*, Carbon, 219 (2024) 118766.
2. A. D. P. Broom *et al*, Applied Physics A, 122 (2016) 151.
3. S. H. Barghi, T. Tsotsis & M. Sahimi, International Journal of Hydrogen Energy, 39 (2014) 1390

Pellet injection in the stellarator TJ-II for fuelling and impurity control studies

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Abstract

The main goal of magnetic confinement fusion research is to establish nuclear fusion as a clean, reliable, secure, and commercially feasible energy source. Stellarator devices are highlighted as promising alternatives to tokamak type designs, offering intrinsic stability and continuous operation potential. However, two critical issues still need to be resolved, i.e., plasma core fueling to overcome the predicted depletion of fuel and impurity accumulation leading to plasma termination by radiation collapse.

The use of cryogenic pellets to fuel large stellarator devices is contributing to the study of long-pulse scenarios for steady operation. Exploring pellet physics on mid-sized machine can offer fresh insights for fuelling on larger devices. For instance, in TJ-II (Spanish stellarator), it is found that the injection of cryogenic hydrogen pellets induces a bifurcation-like transition to a high-performance branch of its fusion triple product, $n_e \cdot T_i \cdot t_E$, when heated using neutral beam injection. This enhanced phase exhibits energy confinement well beyond stellarator ISS04 scaling expectations and, as a consequence, the TJ-II operational regime has been extended. This new scenario in TJ-II can help to better understand the physics underlying fuelling phenomena observed in large stellarators such as W7X (Germany) and LHD (Japan).

Impurity accumulation is the second critical issue that needs to be resolved for the development of steady-state stellarator operation. In this sense, efforts are being made to develop techniques and identify operation scenarios that will avoid impurity accumulation. Experiments are being carried out in TJ-II and LHD to study impurity confinement using the Tracer Encapsulated Solid Pellet (TESPEL) method. This involves the injection of a known quantity of selected impurity tracers encapsulated in a polystyrene capsule into plasma. Current experiments focus on temperature gradient dependence and complementary experiments to deepen understanding.

In this work, a general view of latest results in fueling by cryogenic pellet and impurity confinement by TESPEL injection in TJ-II and LHD will be addressed.

Thermophotovoltaics: fundamental limits and avenues to approach them

1st author

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Abstract

Thermophotovoltaic systems are becoming increasingly more relevant as an approach to harness light for renewable energy that is complementary to solar photovoltaics. Although recent heat-to-electricity conversion efficiencies have already exceeded the Shockley-Queisser limit [1], I will demonstrate that there still exists a large parameter space for further performance enhancement [2]. I will present two distinct approaches for reaching ultra-high conversion efficiencies near the Carnot limit: enabling near-field interactions between the emitter and cell [3] and leveraging hot-carrier photovoltaic cells for harnessing high-energy thermal photons [4]. I will additionally discuss two recently introduced approaches to leverage nonreciprocity for accessing high thermodynamic efficiencies in the case of solar photovoltaics [5] and thermophotovoltaics [6] that rely on tandem photovoltaics. Finally, I will introduce a thermodynamic figure of merit for the universal classification of experimentally demonstrated performances of thermophotovoltaic devices with respect to their thermodynamic limits [7].

[1] Thermophotovoltaic efficiency of 40%, A. LaPotin et al, Nature 604, 287-291 (2022)

[2] Thermodynamics performance bounds for radiative heat engines, M. Giteau, M. Picardi, G. T. Papadakis, Phys. Rev. Applied 20, L061003 (2023)

[3] Thermodynamics of light management in near-field thermophotovoltaics, G. T. Papadakis, M. Orenstein, E. Yablonovitch, S. Fan, Phys. Rev. Applied 16, 064063 (2021)

[4] Hot carrier thermophotovoltaic systems, K. Nimje, M. Giteau, G. T. Papadakis, Journal of Optics, 10.1088 (2024)

[5] Reaching the Ultimate Efficiency of Solar Energy Harvesting with a nonreciprocal multijunction solar cell, Y. Park, B. Zhao, S. Fan, Nano Lett. 22, 448-452 (2022)

[6] Nonreciprocal thermophotovoltaic systems, Y. Park, Z. Omair, S. Fan, ACS Photonics 9, 3943-3949 (2022)

[7] Thermodynamics figure of merit for thermophotovoltaics, M. Giteau, M. Picardi, G. T. Papadakis, Journal of Photonics for Energy, 14, 4 (2024)

Funding

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Catalunya through the CERCA program.

A twist for tunable electronic and thermal transport properties of nanodevices

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Abstract

Twisted graphene-layered materials with nonzero interlayer twist angles (?) have recently become appealing, as they exhibit a range of attractive physical properties, which include a Mott insulating phase and superconductivity. In this study, we consider nanodevices constructed from zigzag graphene nanoribbons with a top rectangular benzenoid [6,3]-flake. Using density functional theory and a non-equilibrium Green's function approach, we explore how the electronic and thermal transport properties in such nanodevices can be tuned through a twist of the top flake by an angle $0^\circ \leq \theta \leq 8.8^\circ$ for different stacking configurations. We found a strong dependency of the electronic structure on the stacking type, as well as on the twisting regime, specifically in AA-stacking devices. Electron and hole van Hove singularities (vHSs), which originate, respectively, from the flatness of the top of the valence band for the minor-spin component and the bottom of the conduction band for the major-spin component, are found very close to the Fermi level in the density of states and electronic transmission spectra of AA-stacking devices with a twist angle of 1.1° . We establish that these vHSs in AA- 1.1° devices are stable at higher temperatures and, with the increased number of available states, lead to larger values of electron thermal conductivity and finally total thermal conductivity in AA- 1.1° . Our work highlights the essential role of twisting and stacking for the fabrication of nanoscale charge and heat switches and spurs future studies of twisted layered structures.[1]

[1] Nanoscale 2024, DOI: 10.1039/D4NR00058G

Modelling light-matter interactions to enhance the performance of advanced halide perovskites based on optoelectronic devices

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Abstract

Halide perovskites show outstanding optoelectronic properties including bandgap tunability or narrow emission lines that make them the optimal candidates for the next generation of solar cells, LEDs and detectors, among other optoelectronic devices.

In this talk we discuss about the optical design of a series of ABX₃ perovskites and their integration in several devices.

We present a transfer matrix-based model powered by a genetic algorithm to extract the complex refractive index of halide perovskites even if they are in device configuration. This tool is critical as their

optical behaviour drastically change depending on the substrate in which perovskites are grown as well as the hole and electron transporting layers between which they are sandwiched, which allows to provide the community with optical constants that are realistic to what the material will show in operando conditions and explains the discrepancies typically attained between optoelectronic response of theoretical designs and experimental trends.

This method enables us to replicate reflectance and transmittance data to elucidate the optical constants of thin film perovskite within a photonic crystal cavity, an integral component of a photodetector device. Once the optical constants are extracted, a comprehensive cavity system can be simulated, incorporating both the photonic crystal and the fitted perovskite layer, to determine the optimal thicknesses of each layer. By doing so, we can simulate resonances within the cavity detector to optimize thicknesses, which results will be presented.

Furthermore, EQE (external quantum efficiency) data can be extracted to determine the optimal current in a triple-junction solar cell device. In this context, we will present a heatmap to optimize the absorption of light in the active layers based on their thicknesses. All calculations are conducted considering the AM 1.5 solar spectrum. This method has improved current matching by almost 2 mA/cm² compared to the experimental device.

Last trends in materials and technologies for next generation batteries

1st author

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Abstract

Research into batteries with better performance, cost and sustainability for applications like electric vehicles or stationary energy storage is a constant both for scientific-technological community and for the industry involved in this sector.

Currently, important advances have been achieved, focused on improving some features of Li-ion batteries, which have allowed this technology to mature technologically and reduce its cost. In this context, different market agents such as Avicenne, IEA, BNEF, or IDtech predict that the main market niche for Li-ion batteries will be the electric vehicle in the coming years with a strong penetration in the near-medium term.

However, batteries continue to face a series of challenges focused on the amount of energy stored, the recharging time, the lifetime, the cost as well as safety and sustainability. The evolution of these battery parameters will be linked to the development of new materials. Those materials will be applied as a cathode, anode and electrolytes in battery cells allowing improvements to current Li-ion batteries or new technologies such as solid batteries, Na-ion, Li-sulfur, metal-air etc. In addition to that, new manufacturing processes and designs of components and cells, and recycling processes for actual and novel technologies will be key points for novel battery technology evolution and market penetration.

Acknowledgements

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Novel TEM tools to shed light into ASSB cathode materials

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Abstract

Cobalt-free, anode-less All Solid-State Batteries (ASSBs), defined as “*Generation 4*” in the *EU Strategic Agenda on Batteries*, are a promising technology due to their safety, longevity, faster charge, environmental impact, application flexibility and potential energy density. However, there are still several constraints in their fabrication, such as the interfacial contact resistance between the components or the stability of the solid electrolytes against Li metal. To assess this last point, advanced TEM techniques provide unique combination of structural and analytical information at multiscale resolutions. In this work, we explore two cathode materials $\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$ and LiFePO_4 , focusing on the structural defects, both arising from fabrication procedures and/or as microstructure evolution in the charge-discharge cycles.

On the one hand, High Resolution TEM has been used for the assessment of crystallinity around grain boundaries, interfaces, and cracks, while quasi-parallel 4D STEM (Scanning TEM), where an electron diffraction pattern is acquired for every pixel, has been used for exploring the texture, local strain, and its influence in the apparition of cracks. On the other hand, Electron Energy-Loss Spectroscopy (EELS) has yielded finer information on local composition around defects. Moreover, two novel paths are explored to tackle the most elusive details of the materials. Firstly, thanks to the application of dimensionality reduction and clustering algorithms the changes in oxidation states of transition metals have been assessed. Secondly, ab-initio simulations by density functional theory and simulation of the free density of states are used to explore the signature of Li throughout the EELS spectrum.

The combination of characterization paths has led to an unprecedented overview of the structure and the changes happening during the charging process in electrodes for all solid-state batteries, paving the path for future in-operando experiments, where the microstructural evolution can be explored in real time.

High performance MXene-based electrodes for energy generation and accumulation storages

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Abstract

Due to the unique properties of 2D MXene materials, they have found their way into a wide variety of applications, including the design of electrochemical devices and a range of other applications. Some of the advantages of these methods are that they can make ultra-thin electrodes that can be used in charge-discharge reactions to reduce the mass of parts that aren't involved. As a result, it is very important that MAX and MXene materials are of the highest quality and capable of delaminating completely in cases such as this. However, often together with single flakes, we have multilayered MXenes particles that also participate in the electrochemical reaction. In this study, we demonstrate the electrochemical behavior of Ti₃C₂ in lithium electrolytes as well as sodium electrolytes upon different steps of the delamination process. MAX phase was obtained by the traditional method using a stainless steel vacuum jar. During the delamination process, different fractions of MXene were sequentially centrifuged and electrodes were subsequently formed from the gradually centrifuged MXene fractions. Electrochemical measurements were carried out using a three-electrode cell with a Pt counter electrode and a Ag/AgCl reference electrode. Based on the results of cyclic voltammetry, impedance spectroscopy and XPS and Raman ex situ studies, it was established that there is a difference in charge accumulation for delaminated and non-delaminated materials. In particular, it has been shown that non-delaminated Ti₃C₂ can provide higher values of capacity at low currents, but during cycling, it has been found that there is a lower value of Coulombic efficiency and a lower capacity retention during cycling compared to an unlaminated Ti₃C₂.

Residual stresses in anode supported BaZr_{1-x}Y_xO_{3-?} electrolytes for solid oxide fuel cells

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Abstract

Yttrium-doped BaZrO₃ (BZY) is a promising candidate as an electrolyte in anode-supported protonic ceramic fuel cells for intermediate temperatures. Proton-conducting fuel cells are typically fabricated in an anode-supported configuration where an electrolyte paste is deposited on the surface of a calcined porous anode pellet and then sintered. The differences in sintering behavior and thermal expansion coefficient can result in the development of elastic residual stresses that can affect the long-term stability of the cell under cyclic operation.

In this work, different sintering conditions, soaking time (5h and 10h), and sintering temperature (1200°C, 1325°C, and 1400°C), were used to fabricate half-cells of BZY₂₀ (BaZr_{0.8}Y_{0.2}O_{3-?}) as the electrolyte and BZY₂₀/NiO as the anode using the solid-state reaction sintering method. The influence of the processing temperature and soaking time on the microstructure, surface finish, and residual stress is proved and shown by detailed XRD and SEM characterization. Rietveld refinement of x-ray diffraction data was used to assess the presence of residual Y₂O₃ and BaY₂NiO₅ in the electrolyte layer as a function of processing conditions, as well as to determine the amount of yttrium incorporated into the perovskite structure through an accurate determination of the lattice parameter. Residual stresses were measured using a specialized diffractometer with an Euler-type cradle and an area detector. Sintering experiments show that a temperature of 1400°C and shorter soaking times may benefit a better formation of the BZY₂₀ structure with larger grain sizes, better surface microstructure, and the presence of compressive residual stresses.

The interface formation challenge in Zero-Excess Solid-State Li Batteries: OPERAndo approaches

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Abstract

Batteries are key elements in modern life and for the transition to a decarbonized economy. However, improved battery technologies are still required to overcome the current limitations of existing Li-Ion Batteries (LIB), concerning safety, energy density and environmental issues related to recycling and to the use of critical materials. Zero-Excess Solid-State Batteries (ZESSB), where the anode is formed in situ at the interface between the solid-state electrolyte and the anode current collector, have emerged as a promising new generation of environmentally friendly batteries with high energy density, and reduced material and cell production costs, moreover simplifying recycling. A remaining key challenge to be addressed is to further improve the homogeneity of the initial anode formation, which has an impact on production costs and battery lifetime. The European OPERA project targets this challenge by a coordinated approach from complementary research fields such as battery technology, surface and material science, synchrotron radiation and multiscale modelling; focusing on operando characterization of the crucial electrolyte-anode interface [1]. The goal is to provide novel information on the influence of stress fields, chemical composition, nucleation and growth kinetics and structural defect formation and to validate the results in model cells. In this talk we will provide an overview of the OPERA project and show detailed results from Low Energy and Photo Emission Electron microscopy (LEEM-PEEM) experiments on Na-ZESSBs performed at the ALBA Synchrotron.

[1] OPERA - Development of operando techniques and multiscale modelling to face the zero-excess solid-state battery challenge, HORIZON Europe Programme, GA 101103834.

Evaluating Ion Beam Techniques and Optical Methods (IBM-OM) to trace H-sorption processes: the magnesium-hydrogen case

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Abstract

Magnesium (Mg) is a plentiful, widely distributed and cost-effective element that can absorb substantial quantities of hydrogen (7.6% wt.). This characteristic renders it a promising candidate for applications in the hydrogen sector [1]. However, certain aspects regarding the thermodynamics and kinetics of the hydrogenation mechanism remain unresolved. To overcome those problems, a precise characterization of the hydrogenation process is needed. In this context, the metal-insulator transition under hydrogen, resulting in significant alterations of its optical properties, makes it suitable for hydrogen optical-sensing in thin films and offers a straightforward way to characterize the hydrogenation process in situ. On the other hand, ion beam techniques present a robust suite of tools for characterization [2], capable of providing detailed depth profiles of hydrogen concentration, thus making them ideal for investigating hydrogenation reactions. In this work, we compared the capabilities of both techniques on tracing the hydrogenation of Pd-capped Mg films under low temperatures (140°C) and hydrogen pressures (1 bar). Whereas IBT revealed the growth of the MgH₂ layer from surface to substrate, OM scarcely detected any changes up until the end of the hydrogenation process. Results provide the reaction mechanism and the H-diffusion coefficient. Finally, the advantages/disadvantages of both techniques (IBT-OM) during H-absorption/desorption reactions will be discussed. Acknowledgements: The authors acknowledge the support from CMAM-UAM for the beamtime (STD005/23, STD020/23) and technical staff support. Laboratorio MiNa (IMN) is acknowledged for the FEG-SEM measurements. Finally, technical assistance of F. Moreno and financial support by Spanish MICINN (PID2021-126098OB-I00/AEI/FEDER10.13039/501100011033) are gratefully acknowledged.

- [1] Aguey-Zinsou, K.F., and Ares-Fernández, J.R., Energy Environ. Sci., 3(5), 526-543, (2010).
[2] A. Redondo-Cubero, M.J.G. Borge, N. Gordillo, P.C. Gutierrez, J. Olivares, R. Perez-Casero and M.D. Ynsa, Eur. Phys. J. Plus 136, 175 (2021)

Plasma Assisted H₂ Production in a Ferroelectric Packed Bed Reactor

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Abstract

Plasma decomposition reactions are used for various gas phase chemical processes including the decomposition of ammonia to generate hydrogen. As an ammonia distribution grid already exists, NH_3 is considered to be the cost-effective carrier enabling in-situ recovery of hydrogen. In this work we show that pure ammonia can be effectively decomposed at atmospheric pressure and ambient temperature using a packed-bed plasma reactor moderated with BaTiO_3 ferroelectric pellets without a catalyst. The decomposition rate and energy efficiency of this ferroelectric barrier discharge reactor have been monitored as a function of applied voltage (up to a maximum value of 2.5 kV) and flow rate. For each operating condition reaction efficiencies have been correlated with the parameters defining the electrical response of the reactor. It is found that plasma current and volume inside the reactor and hence the energy efficiency of the process and the decomposition rate vary with the applied voltage and the flow of ammonia (a maximum decomposition rate of 14% and an energy efficiency of 150 LH_2/kWh has been determined under optimized operation conditions). The role of back reactions (i.e. $\text{N}_2 + 3\text{H}_2 \rightleftharpoons 2\text{NH}_3$) in decreasing reactor performance is another key effect affecting the overall efficiency for the ammonia decomposition. The possibilities of ferroelectric barrier discharge reactors to induce the decomposition of ammonia and the importance of keeping the operating temperature below the Curie temperature of the ferroelectric material are highlighted.

Variation of Pd thickness in Mg/Pd thin films for enhanced hydrogen absorption kinetics

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Abstract

Magnesium has emerged as a compelling candidate for optical hydrogen sensing due to its significant optical response upon hydrogenation, switching between reflective and transparent states. However, thermodynamic and kinetic restrictions as well as its high reactivity hinder its practical use [1]. To overcome these difficulties, Mg-films are usually capped with an ultrathin catalytic layer of palladium (Pd) to reduce the hydrogen dissociation barrier [2] and prevent the formation of oxides/hydroxides onto the Mg-surface. In this work, the role of the palladium thickness (from 1 to 30 nm) on the H_2 absorption process was investigated near ambient temperatures ($T < 80^\circ\text{C}$). For this purpose, Pd-capped Mg films were deposited using e-beam evaporation and structurally and morphologically characterized using X-ray diffraction (XRD), profilometry and field emission gun scanning electron microscopy (FEG-SEM), respectively. The hydrogen absorption process was analyzed “in situ” by optical transmittance measurements. Obtained results show (i) a drastic influence of Pd- thickness on H-kinetics and (ii) a two-step control mechanism (nucleation and

growth and H-diffusion) in the hydrogenation process. Since the explanation of the palladium's influence on H-absorption kinetics is still debated due to the variety of phenomenology involved at film surface/interface, a complete set of characterization techniques were employed to discern the underlying causes for the observed kinetic enhancement. Thermal Desorption-Mass Spectrometry (TD-MS), X-ray Photoemission Spectroscopy (XPS), Scanning Transmission Electron Microscopy-Energy Dispersive Spectroscopy (STEM-EDS) and Electron Energy Loss Spectrometry (EELS) were performed to provide an accurate morphological, structural and compositional characterization of the film's surface and interface. Acknowledgements Technical assistance of F. Moreno and financial support by Spanish MICINN (PID2021-126098OB-I00/AEI/FEDER10.13039/501100011033) are gratefully acknowledged.

[1] K.F. Aguey-Zinsou et al. *Energy Environ. Sci.*, 3, (2010) 526–543.

[2] S. C. Smith et al. *Journal of ACS*, 129 (2007), 10201-10204.

An analytical model for back illuminated electrodes for its application in water splitting photoelectrochemical cells

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Abstract

The deployment of carbon-free energy technologies that could compete with the price of fossil fuels is expected to be a key factor for sustaining the future energy requirements of the world population. Hydrogen is a promising energy vector that can be produced using solar energy. In this regard, tandem photoelectrochemical cells have attracted major attention as devices for green hydrogen (and other fuels) generation in the last years. They are composed of two semiconductor-based electrodes (photoanode and photocathode) illuminated from different sides, which should exhibit complementary characteristics to work under bias-free conditions. [1,2] In this contribution, we present a model for the theoretical prediction of the current-voltage characteristic curves in semiconductor-electrolyte junctions. The theory for charge carrier dynamics in the semiconductor film under light excitation is considered for building up the model equations using as input geometric and physic parameters of the electrode. Recombination in the diffusion-driven region and space-charge region are included. The analysis of limiting cases leads to simplified cases that allow the prediction of the physical properties of the semiconductor under simple experimental analysis in practical photoelectrodes. The model can be integrated into a broader analysis to predict the limits of solar-to-hydrogen efficiencies in photoelectrochemical cells for hydrogen production.

[1] Monllor-Satoca, D.; Díez-García, M. I.; Lana-Villareal, T.; Gómez, R. Photoelectrocatalytic Production of Solar Fuels with Semiconductor Oxides: Materials, Activity and Modeling. *Chem. Commun.* 2020, 56, 12272.

[2] Díez-García, M. I.; Gómez, R. Progress in Ternary Metal Oxides as Photocathodes for Water Splitting Cells: Optimization Strategies. *Sol. RRL* 2022, 2100871.

POSTER: No Production in a Gliding Arc Plasma Reactor.

Presenter

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Abstract

Gliding arc plasma reactors have received much attention lately to carry out certain plasma-assisted chemical processes due to their high efficiency. In this work, we analyze the generation of Nitric oxide (NO) from air using a cylindrical gliding arc plasma reactor. Our investigation focuses on understanding the influence of the reactor operational parameters on the chemical yield and the energy efficiency of the process. NO quantification was carried out using FTIR, and mass spectrometry and energy efficiency calculations were performed to assess the effectiveness of the process in converting electrical energy into chemical products. Gliding-arc plasma discharges were generated between the reactor electrodes by applying voltage drops of different magnitudes and frequencies, and flowing air at a fixed rate of 10 L/min. Our results show that the NO production does not follow a uniform tendency with electrical working parameters, ranging from 15% up to a remarkable 20% of NO production. These promising results provide crucial insights into the overall performance and suitability of gliding arc plasma for NO production. However, the lack of a clear trend prompts further investigation of the underlying physical mechanisms and potential limiting factors.

POSTER: Plasma-Catalytic Dry Reforming of Methane: on the Role of a Ni Catalyst at Room Temperature.

Presenter

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Abstract

Plasma reactions involving $\text{CO}_2 + \text{CH}_4$ mixtures have been proposed as a viable process for the dry reforming of methane. Without specific catalysts, predominant studies report the formation of CO and H_2 as the primary reaction products while when adding catalysts Cn hydrocarbons ($n > 1$) can also be obtained. However, the role of catalysts in plasma-assisted chemical processes at room temperature is currently a matter of debate. Recent studies suggest that the plasma-catalysis synergies observed are not due to a classical catalytic effect but rather to the modifications that the inclusion of catalysts induces in the electrical behavior of the plasma reactors. To address these questions, we investigated the $\text{CO}_2 + \text{CH}_4$ plasma reaction in a ferroelectric-moderated packed-bed reactor, where we varied the reactant ratio, without catalyst and adding a Ni catalyst in the packed-bed barrier. The electrical behavior of the reactor was analyzed in each case and the distribution of reaction products was obtained by using mass spectrometry. Our results reveal that the catalytic effect is second-order when high dielectric constant ferroelectric materials are used as discharge moderators.

POSTER: Revisiting the optical properties of magnesium thin films

Presenter

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Abstract

Magnesium (Mg) is an abundant element that exhibits remarkable optical change due to its optical transition under hydrogen exposure from metallic Mg to dielectric magnesium hydride (MgH_2) becoming very attractive to be utilized in optical switching applications. For developing such applications, it is crucial to accurately determine the optical properties of the films to obtain parameters such as the complex refractive index ($\tilde{n}=n+ik$) or the absorption coefficient (?). Surprisingly, while significant research has been performed on synthesizing and characterizing Mg films there is hardly any explicit work on their optical properties in previous literature [1-2]. To surmount previous inconvenience, Mg films of different thicknesses were deposited using e-beam evaporation. Films were morphologically and structurally characterized by profilometry, scanning electron microscopy (SEM-FEG) and X-ray diffraction (XRD), respectively. Subsequently, ellipsometry and reflectance measurements were performed to analyse the optical properties of the films. Obtained results were interpreted by a novel non-Drude model due the particular morphology of Mg films providing reliable information about the influence of the film morphology on its optical properties.

[1] R. Machorro et al., Thin Solid Films, 269(1-2),1-5. [https://doi.org/10.1016/0040-6090\(95\)06653-5](https://doi.org/10.1016/0040-6090(95)06653-5)

[2] D. Hacman and W. Heitmann, Appl. Opt. 12(4), <https://doi.org/10.1364/ao.12.000895>.

POSTER: Customized Heusler alloys for magnetic refrigeration

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Abstract

In this work, Ni-Mn-(Sn, In) based Heusler alloys with magnetocaloric effect have been produced. Magnetocaloric-based solid-state magnetic refrigeration offers green and sustainable refrigeration with greater efficiency, compactness, and environmental friendliness than conventional gas-compression refrigeration systems. Correct compositional control allows the transformation temperatures to be shifted to the desired temperature range. The minority addition (1 at.%) of a fourth element to the Heusler alloy allows the temperature of the structural transformation (martensitic) to be shifted by about 50 K.

In this study, we are looking for customized alloy candidates for magnetic cooling in data centers. The interest in data centers is because it is estimated that the overall energy consumption due to data centers will reach 4-5% in 2027. One of the energy parameters to be maximized is the refrigeration capacity, RC. On the other hand, cooling processes are cyclic, and it is necessary to study the functional response after cycling. Studies have been carried out after 100 thermal cycles and, it has been found that the effect on thermodynamic parameters (entropy, enthalpy) is a reduction of about 10-12%. This reduction occurs mainly in the first 2-3 cycles and it is related to: a) the accommodation of the martensitic phase and b) the release of the crystallographic defects.

In addition, the heat exchange of these materials was simulated in two configurations. An advantage is that by having experimental results, in the simulation we can use data from our specific nanocrystalline alloys. The calculated coefficient of performance (COP) is higher (for the same temperature range) in magnetic cooling than in conventional refrigeration (about 15%).

POSTER: Hybrid aqueous supercapacitors based on Mxene/activated carbon

Presenter

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Abstract

Increasingly, power sources with high power, good cycling, and high capacity are needed to meet the needs of modern devices. Each electrode of an electrochemical energy device determines the power of the device by the rate of electrochemical reactions that occur there. With a hybrid supercapacitor, the reaction rate is limited by an intercalation-type Faraday electrode. Due to this, the development of novel 2D materials is now of great importance, such as MXenes, which have a large surface area. Moreover, MXenes single flakes remain stable in water for long periods, making them a good material for cheap and

environmentally friendly aqueous supercapacitors. A major focus of our research is on investigating the electrochemical properties of hybrid supercapacitors that are formed on the basis of Ti_3C_2 and activated carbon derived from apricot pits. Electrochemical studies were carried out in coin cells (CR 2032) in 1M aqueous solutions of Na_2SO_4 , NaNO_3 and Na_2CO_3 . The calculation of the specific capacity based on the calculated values of the specific capacity, especially under high current conditions, allowed us to conclude that this combination of electronic materials could be used for hybrid electrochemical systems with a high cycling rate and a high power density. There is a special importance to pay attention to the transformation of the impedance spectra during the cycling process, which indicates the stability of the charge accumulation processes on the two electrodes over the course of a thousand cycles.

POSTER: The Origin of Amphipathic Nature of Short and Thin Pristine Carbon Nanotubes—Fully Recyclable 1D Water-in-Oil Emulsion Stabilizers

Presenter

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Abstract

Short and thin pristine carbon nanotubes (CNTs) emerge as 1D emulsion stabilizers capable of replacing aquatotoxic low-molecular surfactants. However, inconsistencies in understanding of water–solid interfaces for realistic CNTs hamper their individualization-driven functionalities, processability in benign media, and compatibility with a broad-scale of matrices. Pristine CNT processing based on water and inexpensive n-alkanes within a low energy regime would constitute an important step toward greener technologies. Therefore, structural CNT components are quantitatively assessed, placing various CNTs on the scale from hydrophobicity to hydrophilicity. This structural interweave can lead to amphipathicity enabling the formation of water-in-oil emulsions. Combining experiments with theoretical studies, CNTs and CNT emulsions are comprehensively characterized establishing descriptors of the emulsifying behavior of pristine and purified CNTs. They emerge as having hydrophilic open-ends, small number of oxygen-functionalized/vacancy surface areas, and hydrophobic sidewalls and full caps. The interplay of these regions allows short and thin CNTs to be utilized as fully recyclable 1D surfactants stabilizing water/oil emulsions which, as demonstrated, can be applied as paints for flexible conductive coatings. It is also shown how the amphipathic strength depends on CNT size, the pristine-to-oxidized/vacancy domains and the oil-to-water ratios.[1]

[1]Adv. Mater. Interfaces 2023, 2202407

Theoretical and Particle Physics Symposium (DFTP) / *Simposio de Física Teórica y de Partículas (DFTP)*

Organiser

Barabara Alvarez González, Antonio Dobado Gonzalez, Emma Torro Pastor

Symposium abstract

The symposium will consist of three main parts. Firstly, the presentation, by young scientists, of innovative results to which they have contributed in the field of theoretical physics, particle physics, gravitation, cosmology and related topics. On the other hand, two invited talks will take place on topics of special relevance for the division that have appeared during the last year yet to be determined. Finally, a small ceremony will take place to present the awards for the best doctoral theses of recent years awarded by the DFTP.

El simposio constará de tres partes principales. En primer lugar la presentación, por parte de jóvenes científicos de resultados novedosos a los que ellos hayan contribuido en el ámbito de la física teórica, física de partículas, gravitación, cosmología y temas afines. Por otra parte tendrán lugar dos charlas invitadas sobre temas de especial relevancia y actualidad aparecidos durante el último año en los temas propios de la división aún por determinar. Por último tendrá lugar una pequeña ceremonia de entrega de los premios a las mejores tesis doctorales de los últimos años otorgados por la DFTP.

List of abstracts at the symposium

Top quark studies with the CMS detector

1st author

Jorge Ayllón Torresano ICTEA-University of Oviedo **on behalf of the CMS Collaboration**

Abstract

The study of the top quark is a topic of great interest in the field of particle physics. The main production processes with top quarks at the LHC are strong production $t\bar{t}$ (a top quark and an anti-top quark), and electroweak production t -channel (one top quark in association with a light quark), tW (one top quark in association with a W boson), among others. The reasons to study this quark rely mainly on being the most massive particle of the Standard Model, have the chance to decay before hadronising and the value of its Yukawa coupling, and hence, the relation of the top with the Higgs boson.

A preview of the studies regarding the top quark will be presented with data from proton-proton collisions produced in the LHC and recorded by the CMS experiment.

Does dust non-Gaussianity affect constraints on primordial gravitational waves and cosmic structure growth?

1st author

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Abstract

A major challenge in the analysis of Cosmic Microwave Background (CMB) data is posed by the presence of Galactic foregrounds, especially thermal dust emission. Both the search for primordial B-modes and measurements of structure growth rely on foreground modelling, for which most works implicitly assume

that all sky components follow Gaussian statistics. However, we know that this is a poor description for Galactic dust, which, for instance, exhibits non-Gaussian filamentary structure that cannot be reproduced from random Gaussian statistics. In this talk, I will present an in-depth study of whether dust non-Gaussianity can bias searches for primordial gravitational waves using CMB B-modes [1]. In addition, I will discuss the impact it has on CMB lensing reconstruction analysis, with a particular focus on the final Atacama Cosmology Telescope CMB lensing power spectrum measurement and the prospects for improved measurements of structure growth and the unknown neutrino mass.

[1] I. Abril-Cabezas, C. Hervías-Caimapo, S. von Hausegger, B. D. Sherwin and D. Alonso (2024) MNRAS, 527, 5751

Measurements of WZ properties in Run 3 with the CMS detector

1st author

Miguel Obeso Menéndez ICTEA University of Oviedo on behalf of the CMS Collaboration

Abstract

Dibosonic production modes (VV, where V can be either a W or Z boson) hold a crucial role in the understanding of the electroweak sector of the Standard Model as well as its possible extensions. In particular, the WZ process allows to test several theoretical features of interest, such as: charge asymmetries in the initial state, measurement of the polarization fractions for W and Z bosons, and direct access to trilinear gauge couplings.

The properties of the WZ production have been measured in several occasions by both CMS and ATLAS at different energies (5, 7, 8 and 13 TeV) using final states with three leptons, where high precision was achieved thanks to the purity of multileptonic selections. With the beginning of Run 3 in 2022 and the achievement of a new energy frontier in proton-proton collisions at 13.6 TeV at the LHC, the CMS Collaboration is starting their first studies and measurements at this energy limit.

Three and four gluon vertices from quenched lattice QCD

1st author

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Abstract

We report on the evaluation of three and four-gluon vertices in Landau-gauge obtained through extensive lattice QCD calculations.

Over the last twenty years, lattice studies examining the three-gluon vertex have primarily focused on specific kinematic configurations, like the symmetric or soft-gluon scenarios. However, we have broadened our scope to analyze the vertex across a wider range of kinematics, which has led to the observation of a phenomenon known as planar degeneracy. This term refers to the tendency for the leading tree-level form factor to depend predominantly on a symmetric combination of squared momenta. We have delved into the implications of this phenomenon, using it to better understand how both the three-gluon vertex and the corresponding strong coupling behave at low momentum.

The lattice studies of the four-gluon vertex are much more limited from lattice QCD due to the complexity of the tensorial space of the Landau-gauge four-gluon vertex as well as the expected larger statistical noise associated to a four-point Green functions. Relying on the planar degeneracy, we have obtained the one

particle irreducible (1PI) four-gluon vertex, which exhibits a finite suppression in the IR non-perturbative regime.

Making use of both three and four gluon vertices, we define the strong coupling with a slightly different prescription to the typical momentum subtraction schemes and find a strikingly good scaling for different three-gluon kinematics as well as four gluon one, suggesting the existence of a universal gluon coupling at deep IR scales.

A new tracking and vertexing algorithm to search for long living particles at LHCb

1st author

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Abstract

A new algorithm has been developed at LHCb which is able to reconstruct and select very displaced vertices in real time at the first level of the trigger (HLT1). It makes use of the Upstream Tracker (UT) and the Scintillator Fiber detector (SciFi) of LHCb and it is executed on GPUs inside the Allen framework. In addition to an optimized strategy, it utilizes a Neural Network (NN) implementation to increase the track efficiency and reduce the ghost rates, with very high throughput and limited time budget. Besides serving to reconstruct Ks and Lambda particles from the Standard Model, the Downstream algorithm and the associated two-track vertexing is expected to largely increase the LHCb physics potential for detecting long-lived particles during the Run3. The sensitivity for new physics models involving long lived particles are presented in this talk.

Updated results on anual modulation from the ANAIS-112 dark matter experiment

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Abstract

The ANAIS experiment is intended to search for dark matter annual modulation with ultrapure NaI(Tl) scintillators in order to provide a model-independent confirmation or refutation of the long-standing positive annual modulation signal in the low energy detection rate of the DAMA/LIBRA experiment at the Gran Sasso Underground Laboratory (Italy), using the same target and technique. Other experiments exclude the region of parameters singled out by DAMA/LIBRA. However, these experiments use different target materials, so the comparison of their results depends on the models assumed for the dark matter particle and its distribution in the galactic halo. ANAIS-112, consisting of nine 12.5 kg NaI(Tl) modules produced by Alpha Spectra Inc., disposed in a 3×3 matrix configuration, is taking data smoothly with excellent performance at the Canfranc Underground Laboratory (Spain) since August, 2017. Last published results corresponding to three-year exposure were compatible with the absence of modulation and incompatible with DAMA/LIBRA for a sensitivity above 2.5% C.L. New filtering protocols based on machine-learning techniques have allowed to improve the sensitivity and testing the DAMA/LIBRA signal at 5% will be within reach in 2025. Beyond ANAIS-112, the ANAIS+ project operating crystals at low temperature and replacing PMTs by SiPMs is in development. Here, the ANAIS-112 experiment will be described, showing the set-up, analysis and calibration methods and background studies. The latest results will be presented together with future prospects for ANAIS-112 and ANAIS+.

Search for Rare Charm Decays into two Muons

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Abstract

This work describes a search for rare leptonic decays of the D_0 meson using data from the CMS experiment collected during the LHC Run-3 in 2022 and 2023. The study focuses on the search for the process $D_0 \rightarrow \mu^+ \mu^-$ and the measurement of its Branching Fraction (BF). This process, involving flavor-changing neutral currents (FCNC), forbidden at tree level in the Standard Model (SM), is analogous to the $B_s^0 \rightarrow \mu^+ \mu^-$ decay, identified as a golden channel for new physics searches at the LHC, and investigated by LHCb and CMS since the LHC Run 1. The SM predicts a $BF(D_0 \rightarrow \mu^+ \mu^-)$ on the order of 10^{-13} . However, deviations from this prediction could indicate contributions from beyond the SM (BSM) physics, such as loop-mediated processes involving virtual particles that are challenging to observe directly at the LHC energy scales.

Rare charm decays mediated by the $c \rightarrow u$ transition have been less explored compared to $b \rightarrow s$ and $b \rightarrow d$ transitions. To date, the $D_0 \rightarrow \mu^+ \mu^-$ decay has not yet been observed, with the most stringent limit to its BR set by LHCb at 3.5×10^{-7} (95% C.L.), representing four orders of magnitude above the SM prediction. By employing a cascade decay approach ($D^* \rightarrow D_0 \mu^+ \mu^-$, $D_0 \rightarrow \mu^+ \mu^-$), this analysis aims to suppress background and enhance sensitivity to this rare decay mode. The study presented in this contribution utilizes trigger

strategies based on low-mass dimuons and addresses primary backgrounds, such as pion decay and semileptonic B decays.

Preliminary results indicate an improvement in sensitivity with respect to the LCHb published result.

Computing activities at the Spanish Tier-2 for the ATLAS experiment in the LHC Run3 and towards High Luminosity (HL-LHC)

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Abstract

The ATLAS Spanish Tier-2s have more than 18 years of experience in the deployment and development of LHC computing components and their successful operation. The sites are actively participating in, and in some cases coordinating, R&D computing activities in the LHC Run 3 and developing the computing models needed in the HL-LHC period. In this contribution, we present details on the integration of some components, such as HPC computing resources to execute ATLAS simulation workflows; the development of new techniques to improve efficiency in a cost-effective way; and improvements in Data Organization, Management and Access through storage consolidations, the use of data caches, and improving experiment data catalogues, through contributions such as Event Index. The design and deployment of novel analysis facilities using GPUs together with CPUs and techniques like Machine Learning are also presented. ATLAS Tier-2 sites in Spain, are, and will be, contributing to significant R&D in computing and evaluating different models for improving performance of computing and data storage capacity in the LHC High Luminosity era.

Studies on Higgs boson pair production in the bb $\tau\tau$ final state using proton-proton collisions at 13TeV data from the CMS experiment

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Abstract

Recent results from the CMS collaboration on resonant and non-resonant Higgs boson pair production in the final state with two bottom quarks and two tau leptons will be presented. Thanks to its sizeable branching fraction (7.3%), this is one of the main modes to study the Higgs boson self-coupling and an interesting tool to probe physics beyond the standard model at the LHC. The analyses utilize data from proton-proton collisions at a center-of-mass energy of 13 TeV. The analysis requires at least one tau lepton that decays hadronically, and benefits from precise tau identification algorithms developed within the CMS collaboration. Multiple machine learning techniques, including Deep Neural Networks, are employed for signal extraction and object selection. The data are found to be consistent, within uncertainties, with the standard model predictions. Upper limits at 95% confidence level are set on the standard model production cross section, the Higgs boson trilinear self-coupling, and the coupling of two Higgs bosons to two vector bosons. The observed (expected) upper limit at 95% confidence level corresponds to 3.3 (5.2) times the SM prediction for the inclusive HH cross section and to 124 (154) times the SM prediction for the vector boson fusion HH cross section. At 95% confidence level, the Higgs field self-coupling is constrained to be within ± 1.7 and 8.7 times the SM expectation, and the coupling of two Higgs bosons to two vector bosons is constrained to be within ± 0.4 and 2.6 times the SM expectation. The study demonstrates a significant improvement in sensitivity compared to previous CMS analyses. Additionally, recent searches for resonant Higgs boson pair production will be discussed. This effort contributes to the broader goal of probing beyond the standard model theories which predict resonances with large branching fractions in Higgs boson pairs.

Development and application of computational techniques for data analysis of CMS at CIEMAT

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Abstract

The anticipated surge in data volumes from LHC experiments, like CMS, particularly in the High-Luminosity LHC era (planned to start in 2029), requires a reevaluation of data management and processing model. The current strategy for the final steps in a LHC data analysis workflow typically involves data reduction on the Grid infrastructure followed by interactive analysis on physicists' workstations. This model is however under revision currently, assessing its scalability to deal with the HL-LHC expected data scales, as well as its adaptability to adopt new data analysis paradigms (e.g. columnar data analysis). In order to deal with these needs, the so-called Analysis Facilities comes into play, which is a rapidly-evolving concept that is

converging to include dedicated hardware infrastructures and computing services optimized for the effective analysis of large HEP data samples.

This contribution will describe the implementation of the new Analysis Facility model at the CIEMAT institute in Madrid, Spain, aimed at supporting the local CMS experiment community. The contribution will detail the deployment and evaluation of dedicated high-performance hardware, the operation of data staging and caching services to ensure efficient access to CMS physics analysis datasets, and the integration and optimization of a customized analysis framework based on ROOT's RDataFrame and CMS NanoAOD format.

Evaluation of Systematic Uncertainties coming from the application of ML/DL methods in the search for $t\bar{t}b\bar{b}$ resonances in the ATLAS experiment (CERN)

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Abstract

The main goal of this contribution is the implementation and verification of procedures for evaluating systematic uncertainties associated with the application of Machine Learning/Deep Learning Methods. The starting point is the results previously obtained for a signal/background classification problem from datasets of simulated events. In order to control the whole performance using several metrics (Accuracy, F1-score, Kappa, AUC,...). These studies have provided promising results. The Physics Analysis context is the search for $t\bar{t}b\bar{b}$ resonances at ATLAS experiment which is a Beyond the Standard Model case under study. In this point the evaluation of the systematic errors is needed. This is performed in two ML/DL methods: in the application of Decision Trees (Boosted Decision Trees and Random Forest) and in the framework of Artificial Neural Networks, where the greatest complexity will be revealed in the case of the second one.

Micromegas detectors for rare event searches in CAPA

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Abstract

Gaseous Time Projection Chambers (TPCs) with Micromegas pixelated readouts are being used in dark matter searches and other rare event searches, due to their potential in terms of low background levels, energy and space resolution, gain, and operational stability. Moreover, these detectors can provide precious features, such as topological information, allowing for event directionality and powerful signal-background discrimination. The Micromegas technology of the microbulk type is particularly suited to low-background applications and is being exploited by detectors developed at the “Centro de Astropartículas y Física de Altas Energías” (CAPA) of the University of Zaragoza and used in experiments like IAXO and TREX-DM.

IAXO (International AXion Observatory), successor of the CAST (CERN Axion Solar Telescope), is a proposed new-generation axion helioscope aiming at a sensitivity much improved with respect to past solar axion searches. BabyIAXO is intended to develop the required magnet, optical and detection systems but having a real discovery potential; it will be installed at DESY.

TREX-DM (TPC for Rare Event eXperiments-Dark Matter) aims at the direct detection of low-mass Weakly Interacting Massive Particles (WIMPs) by operating a gas TPC read with Microbulk Micromegas at the Canfranc Underground Laboratory.

Both projects share challenges like the reduction of intrinsic background levels and technical issues like robustness of detector, new design choices or scaling up to larger detector sizes. Here, IAXO and TREX-DM experiments will be described and the status, prospects of the development ongoing and sensitivity will be discussed.

Lepton Flavour Universality tests with b-baryon decays at the LHCb experiment

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Abstract

Rare $b \rightarrow s \ell^+ \ell^-$ transitions are strongly suppressed in the Standard Model (SM). Leptons from the different families have the same coupling to electroweak bosons in the SM, symmetry that is known as Lepton Flavour Universality. Precise measurements of LFU ratios in $b \rightarrow s \ell^+ \ell^-$ decays provide, then, a very powerful test of the SM. RpK was the first LFU test involving b-baryons published by LHCb, which studies the decay $\Lambda_b \rightarrow p K^- \ell^+ \ell^-$ using Run 1 and 2016 data and yielded a compatible result with the SM within 1 standard deviation significance, as well as the first observation of the $\Lambda_b \rightarrow p K^- e^+ e^-$ decay. The new RpK analysis includes full dataset (adds 2017-18 data), a full re-optimisation of the selection after the observation of the electronic decay, with particular focus on the MVA and particle identification requirements. Additionally, the measurement splitted in low and central q^2 regions will be provided, together with the result of the decay into the lightest resonance of $p K$, $\rho(1520)$.

Classical and Quantum higher-order superintegrable momentum-dependent Hamiltonians on curved spaces from the Zernike system

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Abstract

We consider the classical momentum- or velocity-dependent two-dimensional Hamiltonian given by
$$\mathcal{H}_N = p_1^2 + p_2^2 + \sum_{n=1}^N \gamma_n (q_1 p_1 + q_2 p_2)^n,$$
 where q_i and p_i are generic canonical variables, γ_n are arbitrary coefficients, and $N \in \mathbb{N}$. For $N=2$, being both γ_1, γ_2 different from zero, this reduces to the classical Zernike system. We prove that $\mathcal{H}_N$ always provides a superintegrable system (for any value of γ_n and N) by obtaining the corresponding constants of the motion explicitly, which turn out to be of higher-order in the momenta. Such generic results are not only applied to the Euclidean plane, but also to the sphere and the hyperbolic plane. In the latter curved spaces, $\mathcal{H}_N$ is expressed in geodesic polar coordinates showing that such a new superintegrable Hamiltonian can be regarded as a superposition of the isotropic 1D curved (Higgs) oscillator with even-order anharmonic curved oscillators plus another superposition of higher-order momentum-dependent potentials.

Furthermore, the symmetry algebra determined by the constants of the motion is also studied, giving rise to a $(2N-1)$ th-order polynomial algebra. As a byproduct, the Hamiltonian $\mathcal{H}_N$ is interpreted as a family of superintegrable perturbations of the classical Zernike system. Finally, it is shown that $\mathcal{H}_N$ (and so the Zernike system as well) is endowed with a Poisson $\mathfrak{sl}(2, \mathbb{R})$ -coalgebra symmetry which would allow for further possible generalizations that are also discussed.

Finally we will discuss the possible generalization of the quantum superintegrable Zernike system.

Casimir energy in 2+1 non-abelian gauge theories

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Abstract

One of the main open problems in particle physics is the analytical derivation of the mass gap in Yang-Mills gauge theories. It is one of the famous Millennial mathematical problems. The solution of this puzzle, is also fundamental for a proper description of QCD. In recent years, some progress has been achieved in the case of 2+1 dimensions by means of reparametrizing the gauge fields in terms of scalar fields that describe the real physics degrees of freedom [1, 2].

We do not know the structure of the quantum vacuum but we can infer some of its properties by perturbing the system confining the gauge fields between two walls, that generates a dependence of the renormalized vacuum energy on the boundary conditions of the gauge fields. Indeed, the behaviour of the corresponding Casimir energy can shed some light on the ultimate structure of the gauge quantum vacuum. The behaviour of the Casimir energy for a massive scalar field exhibits exponential decay which is proportional to the product of the mass m and the distance between the walls L . However, the coefficient in front of this exponential decay depends of the type of boundary conditions of the fields. This

dependence, can be used to check the coincidence of the Casimir energy of the gauge theory with that of an effective massive scalar field [3, 4].

In this work, we elaborate this argument by numerically computing the Casimir energy for a 2+1 SU(2) gauge theory using lattice simulations, and compare the results with those of the massive scalar field, in a variety of boundary conditions [5]. The results provide a robust test of the conjecture that the infrared behavior of gauge theories is governed by an effective scalar fields with a mass which is much lower than the glueball mass.

[1] Karabali, D. Kim, C.; Nair, V. Planar Yang-Mills theory: Hamiltonian, regulators and mass gap. 352 Nuclear Physics B 1998, 524, 661–694.

[2] Karabali, D.; Nair, V. On the origin of the mass gap for non-Abelian gauge theories in $(2+1)$ dimensions. Physics Letters B 1996, 1, 141–147.

[3] Chernodub, M.N.; Goy, V.A.; Molochkov, A.V.; Nguyen, H.H. Casimir Effect in Yang-Mills 348 Theory in $D = 2 + 1$. Physical Review Letters 2018, 121, 191601.

[4] Karabali, D.; Nair, V.P. Casimir effect in $(2+1)$ -dimensional Yang-Mills theory as a probe of the magnetic mass. Physical Review D 2018, 98, 105009.

[5] Asorey, M.; Ezquerro, F.; Iuliano, C. Casimir energy in 2+1 dimensional field theories. Physics 2024, 6(1)

Enhanced Particle Identification in the LAGO Water Cherenkov Detectors Network through Machine Learning Techniques

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The LAGO Collaboration The LAGO Collaboration

Abstract

Addressing the complex nature of transient astrophysical phenomena and space weather events, the Latin American Giant Observatory (LAGO) stands as a ground-based observatory equipped with a network of Water Cherenkov Detectors (WCDs). These detectors are instrumental for measuring the flux of secondary particles derived from astroparticles impinging the Earth's atmosphere, with limited capability to classify these secondary particles into electromagnetic and muonic groups. The analysis of discrete signals generated when particles traverse a Water Cherenkov Detector (WCD) are indicative of the particle's identity through the specific response of the detector. The resulting charge distribution histograms are the main tool for extracting information about the nature of secondary particles. However, significant challenges persist in effectively resolving the contributions of various secondary particle types. To address this, our approach extends prior research using OPTICS, a density-based clustering algorithm and a type of

unsupervised machine learning method to group and identify different particle types. This technique exploits the WCDs' differential response to particles and enables accurate determination within the secondary particle flux. This work validates the proposed method through the analysis of simulated data, showing a high confidence in its capability of accurately grouping the different secondary particle types. This dataset was created by integrating outputs from the ARTI and MEIGA frameworks, emulating the WCD signal response to secondary particle flux over a day at the LAGO site in Bariloche, Argentina. We integrated real-time magnetospheric and local atmospheric conditions from early 2012 into a Geant4 model of the WCD, adapted by MEIGA for our analysis. The success of this approach shows its potential for applying such machine learning models at the edge of the LAGO detector network, advancing towards onboard real-time data analysis on remote sites. This methodology can be easily adapted to other experiments utilising WCDs as HAWC, Auger, IceTop, and SWGO.

In-situ jet calibration in the ATLAS experiment

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Abstract

The jet response and its uncertainties are key to precision measurements and searches at the LHC. In this presentation, an overview is given of the in-situ jet calibration in the ATLAS experiment. To calibrate the jet p_T response, collision data is used for processes where a jet recoils against a reference system with a well-measured transverse momentum, like a leptonically decaying Z-boson, or a photon. The mass response of groomed large-radius jets is calibrated using the mass peaks of highly boosted W-bosons and top quarks. Results from the run 2 calibration are presented, with emphasis on recent developments.

Status of the Short-Baseline Near Detector neutrino experiment at Fermilab

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Abstract

The Short-Baseline Near Detector (SBND) is one of three Liquid Argon Time Projection Chamber (LArTPC) neutrino detectors positioned along the axis of the Booster Neutrino Beam (BNB) at Fermilab, as part of the Short-Baseline Neutrino (SBN) Program. The detector is currently being commissioned and is expected to take neutrino data this year. SBND is characterized by superb imaging capabilities and will record over a million neutrino interactions per year. Thanks to its unique combination of measurement resolution and statistics, SBND will carry out a rich program of neutrino interaction measurements and novel searches for physics beyond the Standard Model (BSM). It will enable the potential of the overall SBN sterile neutrino program by performing a precise characterization of the unoscillated event rate, and constraining BNB flux and neutrino-argon cross-section systematic uncertainties. In this talk, the physics reach, current status, and future prospects of SBND are discussed.

NuESS, a new opportunity for CEvNS at the ESS

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Abstract

The recent detection of the coherent elastic neutrino-nucleus scattering (CEvNS) opens the possibility to detect neutrinos with small-size detectors and with different techniques, opening a new window to explore possible BSM physics.

The CEvNS process generates signals at the few-keV level, requiring sensitive detection technologies for its observation. The European Spallation Source (ESS) has been identified as the best possible site for the exploration this CEvNS process.

Within the NuESS program, two different detector approaches are currently under development at Donostia International Physics Center (DIPC). The GanESS project, a high-pressure gaseous time projection chamber (TPC) and the CoSI project, which employs cryogenic undoped CsI crystals.

These next-generation technologies will be capable of observing the process with lower energy threshold and better energy resolution than current detectors. In addition, the combination of these detectors will allow for a complete phenomenological exploitation of the CEvNS signal. In particular, these measurements will not be statistically limited due to the synergy between larger neutrino fluxes at the ESS and these improved detectors.

I will give an overview of the current status of NuESS with a focus on its short-term plans.

The GanESS experiment: CEnuNS detection with high pressure noble gas TPCs

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Abstract

This abstract details advancements in neutrino detection technology at the European Spallation Source (ESS) through innovative gaseous detectors made to study coherent elastic neutrino-nucleus scattering (CEnuNS) interactions. Neutrinos, elusive particles with negligible mass and no charge, hold significant detection challenges, and the GanESS experiment, which stands for Gaseous Detector for Neutrino Physics

at the ESS, is meant to detect this interaction using relatively light detectors and explore physics beyond the Standard Model.

The detection concept consists of a high-pressure gaseous time projection chamber (TPC), which will allow us to have a low energy threshold, potentially as low as 1-2 e-. It will use the electroluminescence process to amplify the while preserving resolution. Moreover, GanESS will be able to operate with different noble gases, such as Xenon, Argon, or Krypton.

Currently, we are working on the Neutrino Lab at the Donostia International Physics Center. The Gaseous Prototype (GaP) at the DIPIC will test the operation at high pressure (up to 50 bar) and with different gases. So far it has been tested in Argon up to 10 bar. GaP will also be used to characterize the response to nuclear recoil at low energies.

Monte Carlo simulations using Geant4 have been utilized to analyze the detector's light response. In this poster, we will characterize the light response of the detector using different sensors: SiPMs and PMTs. We will also compare the obtained data with the experimental results obtained so far.

Women in Physics (GEMF) / Mujeres en Física (GEMF)

Organiser

Board of directors GEMF (Junta de Gobierno del GEMF)

Invited speakers

Lorena Fernández, Director of Digital Identity at the University of Deusto.

Symposium abstract

The GEMF symposium will aim to debate topics that have to do with strategies to increase the presence of women in physics, make their achievements visible and defend the interests and equal rights and opportunities of physicists.

El simposio del GEMF tendrá como objetivos debatir temas que tengan que ver con estrategias para aumentar la presencia de mujeres en física, visibilizar los logros de éstas y defender los intereses y la igualdad de derechos y oportunidades de las físicas.

List of abstracts at the symposium

De aquellos sesgos, estos algoritmos

1st author

Lorena Fernández University of Deusto

Abstract

La Inteligencia Artificial (IA) y los algoritmos moldean la sociedad que nos rodea. Deciden a qué información accedemos, qué música escuchamos, qué series vemos, cómo respondemos a un email, qué burbuja ideológica nos rodea, si nos conceden un préstamo... Y hemos metido esos algoritmos en hospitales, colegios, comisarías, nuestras casas y, por supuesto, nuestro bolsillo.

¿Qué sabemos de ellos? Poco o nada. Son opacos, invisibles a nuestros ojos (a la par que esenciales). El gran gol que nos ha metido la tecnología es hacernos pensar que es neutra y que las decisiones que tome serán mejores al no estar sujeta a condicionamientos humanos... y no siempre es así. Está cargada de sesgos de género, raciales, de orientación sexual... De hecho, en muchas ocasiones son sistemas que replican y amplifican esos sesgos, dado que hoy en día son un vehículo primordial de transmisión cultural y de conocimiento y están creando "verdades algorítmicas" irrefutables que refuerzan un modelo único.

¿Y cómo puede suceder esto si son ceros y unos no sujetos a emociones? La inmensa mayoría de las aplicaciones de Inteligencia Artificial en la actualidad se basan en la categoría de algoritmos de deep learning que establecen patrones tras procesar grandes cantidades de datos. Es decir, son como estudiantes en un colegio: aprenden del libro de texto (información con la que se les entrena para que generen reglas de inferencia) y del profesorado (que es quien decide qué temas entrarán en el examen... y le dice a su alumnado, por tanto, qué parámetros son importantes). En esta ponencia analizaremos en qué puntos y de qué manera se pueden cargar de sesgos, cuáles son las causas y cómo podemos resolver esto.

La tecnología nos hace dar pasos hacia adelante, pero para ello debe ser inclusiva y diversa. Hagamos que aquellas personas y colectivos que han sido históricamente marginalizados tengan la oportunidad de decidir y construir sus propios futuros sociotécnicos dignos.

Traces and trails: professors of atomic, molecular and nuclear physics in Spain

1st author

Marta Seror CSIC

Abstract

The difference in participation of women in science is especially evident in higher spheres of teaching and research, positions in which they are scarce. In Spain, the number of female professors of all areas in university has remained unchanged over the past years at around 25%, being even lower in STEM areas. In the case of Physical Sciences, this proportion reaches only 15%. In the Master's thesis of this contribution's name, a series of calculations have been made on the basis of the Ministry of Universities database. Further analysis indicates that, among the variety of Physics disciplines, the percentage of female professors of Atomic, Molecular and Nuclear Physics is the highest at a national level: 22,39% (2021-2022). In order to outline the reasons for this apparent uniqueness, some factors that favor balance in science were examined, with a focus on this experimental science. Based on a set of interviews with active and retired female professors from public universities in Spain, this paper looks at the extent to which gender has or has had an impact on their scientific careers and academic trajectories. In addition to the testimonies collected, another purpose of the study is to locate and highlight female professors in this discipline. The characteristics of this branch of knowledge make the physics of the very small a field in which women have played and continue playing a particularly relevant role.

Gender dynamics in class participation: insights from higher education in Physics

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Abstract

The gender expectations significantly shape the dynamics of participation in higher education; there is a discrepancy in participation between men and women. Women tend to ask fewer questions than men, reflecting social norms that prioritize obedience and non-disruptive behavior in women. Conversely, men often engage in more explanatory discourse, aligning with gender stereotypes that value confidence and competitiveness. This communication presents the study conducted at the Faculty of Physics of the University of Barcelona during the 2022-2023 academic year with students from first to fourth grade. We have investigated the participation in class from a gender perspective, employing a mixed design encompassing quantitative observations (n=900) and, for the qualitative part, a focus group discussion. Our study finds gender disparities in class participation: as expected, women speak less. Interestingly, this effect is moderated in classes where gender ratios are more balanced or when groups are smaller. Teacher gender seems to play no significant role in gendered student participation. Regarding the type of participation, women predominantly answer questions, while men amplify the information given in class or correct the teacher more often, in accordance with established gender mandates. For students, feelings associated with participation tend to be fear and insecurity. In this sense, although most students do not perceive the rest of the student body as a hostile, it is observed that some male students tend to reinforce this emotional tone in class by trying to appear knowledgeable and snubbing other students.

Gender approach in university teaching: activities of the Grupo de Innovación Docente Multidisciplinar para a Igualdade de Xénero (GIDMIX)

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Abstract

Gender-sensitive teaching can improve the quality and social relevance of knowledge, technologies, and innovations produced. It can also stimulate critical thinking and develop skills that enable students to avoid gender blindness in their future professional practice. However, diagnoses of the degree of integration in classrooms reveal disparities between universities and, in general, partial integration. The causes identified include the absence of teacher training in gender issues and the lack of methodological guides on how to introduce the gender dimension, as well as practical examples of how to implement it in different subjects. This is especially important for science and technology subjects. While it is often argued that the content is abstract or highly technical and therefore gender-neutral, this ignores the fact that gender mainstreaming applies not only to the content taught but also to the way it is taught. Therefore, it is crucial to pay attention to non-sexist and non-androcentric language, introduce female references, manage the classroom in an inclusive way, and carefully word exercises and their contextualisation to avoid perpetuating gender stereotypes. This paper presents the activities of the Grupo de Innovación Docente Multidisciplinar para a Igualdade de Xénero (GIDMIX), a Consolidated Teaching Innovation Group recognized by the University of A Coruña. The premise of our activities is that all subjects can include a gender perspective, although the depth of this will vary according to the field of knowledge and the subject of the degree. The experience of GIDMIX members as teachers in physics, engineering, architecture, and econometrics has enabled the development and implementation of gender perspective activities in their subjects. These activities can serve as examples for other teachers to reflect on their own subjects and implement gender perspective in their classrooms.

Fortaleciendo la igualdad y la diversidad en el Instituto de Física de Cantabria

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Abstract

La comisión de igualdad y diversidad del IFCA (CSIC-UC) fue creada en 2020 por la dirección del instituto tras varios años de desarrollo de acciones de igualdad de género realizadas de forma voluntaria por un grupo de investigadoras del centro e impulsado por Teresa Rodrigo. Dicha labor permitió al centro la obtención del accésit del distintivo de igualdad concedido por el CSIC en 2018. El trabajo de la comisión fue también galardonado con el VI premio a la Igualdad de la Universidad de Cantabria en 2022.

El principal objetivo de esta comisión es incluir la perspectiva de género y diversidad en el desarrollo diario de la labor científica del IFCA. Para ello la labor de la comisión se ha centrado desde su creación en tres pilares: coordinar un diagnóstico de la situación del centro en términos de sesgos y discriminación e implementar las medidas adecuadas para asegurar el cumplimiento de los objetivos marcados; formar en igualdad en las carreras STEM; y difundir la ciencia con perspectiva de género y diversidad para el público en general y en particular a estudiantes de educación primaria y secundaria.

En esta charla, presentaremos un resumen de las principales actividades realizadas por esta comisión desde su creación así como las lecciones aprendidas en este camino.

English (version)

The IFCA (CSIC-UC) equality and diversity commission was created in 2020 by the institute's management after several years of developing gender equality actions carried out voluntarily by a group of female researchers at the centre and promoted by Teresa Rodrigo. This work enabled the centre to obtain the second prize of the CSIC equality award in 2018. The work of the commission was also awarded the VI Equality Award of the University of Cantabria in 2022.

The main objective of this commission is to include the gender and diversity perspective in the daily development of IFCA's scientific work. To this end, the work of the commission has focused since its creation on three pillars: coordinating a diagnosis of the situation of the centre in terms of bias and discrimination and implementing appropriate measures to ensure compliance with the objectives set; training in equality in STEM careers; and disseminating science with a gender and diversity perspective to the general public and in particular to primary and secondary school students.

In this talk, we will present a summary of the main activities carried out by this commission since its creation as well as the lessons learned along the way.

Tornem als instituts: actividades de visibilización de las mujeres en los estudios de Física

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Abstract

En esta comunicación presentamos la actividad “Tornem als instituts” realizada por estudiantes de la Facultat de Física de la Universitat de València en los cursos 22/23 y 23/24 y supervisada por las profesoras de la Comissió d'Igualtat. Esta iniciativa, que nace para conmemorar el 11 de febrero, Día Internacional de la Mujer y la Niña en la Ciencia, se planteó dos objetivos de partida: en primer lugar, potenciar las vocaciones científicas, en particular hacia la Física, de las alumnas de los últimos cursos de la secundaria obligatoria; y en segundo lugar, dar formación en relaciones de género al alumnado de nuestra facultad. La

actividad consiste en la realización de charlas divulgativas en centros de educación secundaria, siendo las ponentes estudiantes de la facultad y los centros educativos destinatarios, aquellos en los que ellas mismas estudiaron.

En cifras, “Tornem als instituts” ha tenido muy buena acogida: en las dos primeras ediciones se inscribieron en la actividad un total de 45 estudiantes, 40 mujeres y 5 hombres, y se han realizado charlas divulgativas en 34 centros repartidos por las tres provincias valencianas. El formato de las actividades ha sido flexible para ajustarse a las preferencias de las ponentes y las necesidades de los centros, predominando las charlas con demostraciones experimentales por ser más interactivas. La estimación de alumnado receptor de estas charlas ronda los 3.500 estudiantes.

En conclusión, la actividad que aquí exponemos nos ha permitido, en primer lugar, acercar la Física y los estudios científicos a un número grande de potenciales futuras estudiantes partiendo de la experiencia de las propias alumnas de la facultad que, por proximidad en edad, resulta más cercano y efectivo. Por otro lado, la organización y preparación de las actividades nos ha permitido estrechar la relación entre estudiantes y profesoras de la facultad.

Proyecto Meitner - Recordando a las pioneras de la Física Nuclear y de Partículas

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Abstract

Proyecto Meitner es una iniciativa de divulgación científica impulsada por el Instituto de Física Corpuscular (IFIC) del CSIC y la Universitat de València con el objetivo de recuperar y poner en valor la contribución de las grandes pioneras de la Física Nuclear y de Partículas a través de la figura de Lise Meitner. Este proyecto, que combina la ciencia con disciplinas artísticas, incluye actividades tan diversas como una obra de teatro, unas jornadas de ciencia y género, un programa de mentoría docente, un concurso de ciencia y arte, vídeos en redes sociales y mucho material didáctico para dar visibilidad a las mujeres en ciencia, acercando científicas del pasado y del presente en Física Nuclear y de Partículas a todos los públicos. Y todo con el fin de promover la igualdad social y la cultura científica, fomentar vocaciones científicas y poner de manifiesto las barreras legales, culturales, históricas y sociales a las que las mujeres científicas se han enfrentado a lo largo de la historia.

Proyecto Meitner ha recibido la subvención de organismos como la FECYT, el CSIC, la Universitat de València o la Diputación de Valencia, y ha sido galardonado en 2023 con el segundo premio Alianza STEAM por el talento femenino del Ministerio de Educación y Formación Profesional.

Mujeres científicas con andares de gigantes

1st author

María Matilde Ariza Montes IES "Pedro Espinosa"

Abstract

INTRODUCCIÓN

La invisibilidad de las mujeres en la ciencia a lo largo de la historia ha ido acompañada de la imposibilidad de acceder a la educación. Su incursión en la enseñanza primaria, luego secundaria y más tarde superior, unida al pensamiento feminista, catapultó a la mujer al derecho a la formación universitaria y, por tanto, a la posibilidad de expresar sus propias ideas en foros antes copados por el hombre. Poder tomar decisiones en contextos científicos ha permitido que la mujer haya jugado un papel muy importante en el desarrollo y la mejora de la ciencia, aunque muchas veces, no ha sido visibilizada esta labor.

Con la propuesta didáctica que aquí se presenta, se quiere poner en valor la participación de la mujer en la mejora de la ciencia, así como promover la sensibilización en género y en igualdad en los centros educativos.

Esta exploración intenta visibilizar perfiles femeninos del mundo científico para que el alumnado descubra referentes en campos como la física, fomentando así las vocaciones científicas desde las edades más tempranas.

PROCEDIMIENTO Y RESULTADOS

En este trabajo, se ha procedido a la búsqueda de cientos de mujeres de relevancia nacional e internacional por sus logros en ciencia y, en segundo lugar, se han seleccionado por sus actuaciones, que han sido merecedoras del protagonismo del que gozan en el campo de la ciencia. Además, se han elegido por los reconocimientos otorgados por parte de las instituciones y de la sociedad en general, así como por los logros científicos y sociales conseguidos gracias a su labor.

Con todas estas características, se ha creado un banco de datos que ha permitido definir cada uno de los perfiles destacados, con la idea de editar un libro sencillo en el que las más jóvenes fácilmente tengan referencias reales de mujeres, que participan en profesiones y actividades de la ciencia, impulsando, por tanto, la paridad, la igualdad y la equidad.

Quantum Optics and Nonlinear Optics Symposium (GEOCONL, GELUR) / *Simposio de Óptica Cuántica y Óptica No Lineal (GEOCONL, GELUR)*

Organiser

Carlos Hernández-García

Invited speakers

Allan Johnson (IMDEA Nanoscience) Rocío Borrego-Varillas (Istituto di Fotonica e Nanotecnologie-consiglio Nazionale delle Ricerche) Guillermo Muñoz Matutano (Universitat de Valencia)

Symposium abstract

The symposium is organized by the Quantum Optics and Nonlinear Optics Group (GEOCONL) in collaboration with the Ultrafast Lasers Group (GELUR) of the RSEF. Oral and poster communications will be presented. It is dedicated to theoretical and experimental developments in the study of the nature of light and its interaction with matter, when quantum and/or nonlinear optical phenomena occur. It includes quantum states of light, cold atoms and matter waves, plasmonics, nanophotonics, coherence effects, physics of lasers and amplifiers, nonlinear and multi-photon processes, strong field physics, nonlinear materials, nonlinear metamaterials, nonlinear photonics crystals, nonlinear spectroscopy, nonlinear dynamics, ultrafast phenomena, generation and characterization of ultra-short and/or ultra-intense light pulses, high harmonic generation and attosecond physics, optomechanics, applications of quantum phenomena and nonlinear photonics.

El simposio está organizado por el Grupo Especializado de Óptica Cuántica y Óptica No Lineal (GEOCONL) en colaboración con el Grupo Especializado de Láseres Ultrarrápidos de la RSEF. Las comunicaciones podrán ser orales o póster. El simposio está dedicado a los desarrollos teóricos y experimentales en el estudio de la naturaleza de la luz y su interacción con la materia, prestando especial atención a los fenómenos ópticos cuánticos y/o no lineales. La temática del simposio incluye estados cuánticos de luz, átomos fríos y ondas de materia, plasmónica, nanofotónica, efectos de coherencia, física de láseres y amplificadores, procesos no lineales y multifotónicos, física de campos intensos, materiales no lineales, metamateriales no lineales, cristales fotónicos no lineales, espectroscopia no lineal, dinámica no lineal, fenómenos ultrarrápidos, generación y caracterización de pulsos de luz ultracortos y/o ultraintensos, generación de armónicos de orden alto y física de attosegundo, optomecánica, aplicaciones de fenómenos cuánticos y fotónica no lineal.

List of abstracts at the symposium

Few-femtosecond coupled charge and lattice dynamics in an ultrafast phase transition

1st author

Allan Johnson IMDEA Nanoscience

Abstract

Ultrafast spectroscopy is an emerging approach for understanding the underlying physics of quantum materials, those systems whose strong couplings between different degrees of freedom makes their theoretical description challenging. Studies often focus on the picosecond or slower timescales because the emergent phenomena in quantum materials often occur at lower energy scales where contributions of the electronic, lattice and spin degrees of freedom are comparable. Here I will show that the process of ultrafast phase transition is an exception, in which the overall symmetry change of the system may launch motion faster than the characteristic frequencies of the quasiparticles, down to the few-femtosecond scale. Using few-femtosecond pulses generated from high-energy solitons spanning the entire deep ultraviolet to infrared (210-2500 nm) we excited and probe the light-induced insulator-to-metal phase transition inside the prototypical quantum material vanadium dioxide (VO₂). Using the ultra-broadband probe we reconstruct the electronic structure at each time delay, and show the system promptly transforms in a bad-

metal state in less than 10 fs, supporting a Mott-like mechanism for the transition. However, this rapid change then launches coherent lattice motion at the sub-100 fs timescale, and we see evidence for structure revivals of the initial phase, including a partial re-opening of the bandgap induced a transient semi-metallic state, before the system thermalizes by 100 fs. Our results show the potential for ultrafast phase transitions to show surprising complexity, with effects analogous to conical intersections in molecular systems and highly non-linear coupling effects. Technically, our high-energy soliton based approach is especially promising as it enables few-to-sub-femtosecond spectroscopy in the optical frequency range at photon fluxes orders of magnitude higher than with conventional attosecond sources, and will enable few-femtosecond spectroscopy in a wide range of quantum materials.

Talbot high-order harmonic spectroscopy from solids

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Abstract

High-order harmonic generation (HHG) is a cornerstone technique for producing attosecond x-ray coherent radiation as well as a remarkable tool for studying the ultrafast dynamics in matter. While extensively studied in atomic and molecular gases, recent attention has shifted towards HHG from solid targets. In the atomic and molecular cases, HHG operates through a three-step model, involving tunnel ionization, acceleration by the laser field, and rescattering with the parent ion, culminating in the emission of high-frequency radiation in the form of harmonics. In the case of solids, the mechanism for HHG differs substantially in the bulk case, when the electron motion is confined into the crystal, or in surface, where the electron is detached from the crystal when the driving field polarization is perpendicular to the surface [1].

HHG from two-dimensional (2D) solids at grazing incidence presents a paradigmatic example of surface-mediated HHG. The ionized wavefunction is structured by the crystal geometry in a periodic pattern, and follows a free electron evolution driven by the field, a situation bears resemblance to coherent optics phenomena [2] like Talbot imaging, applied to matter waves. In this contribution we examine the interaction of few-cycle mid-infrared laser pulses with one-dimensional crystals at grazing incidence, depicting the HHG process affected by Talbot-like modulations in the ionized electronic wavefunction. Most remarkably, the spatio-temporal scale of the phenomena (nanometers and femtosecond) found is unprecedented in other Talbot studies, and its relevance for HHG allows us to coin ultrafast Talbot spectroscopy as a new pathway for the study of matter at the smallest spatial and shorter time scales [3].

[1] N. Tancogne-Dejean and A. Rubio; Sci. Adv., 4, eaao5207 (2018).

[2] C. Granados and L. Plaja; Phys. Rev. A, 89, 023428 (2014).

[3] A. García-Cabrera, C. Hernández-García and L. Plaja; New J. Phys., 23, 093011 (2021)

A mixed perturbative-nonperturbative treatment for strong light-matter interactions

1st author

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Abstract

The full information about the interaction between a quantum emitter and an arbitrary electromagnetic environment is encoded in the so-called spectral density. We present an approach for describing such interaction in any coupling regime, providing a Lindblad-like master equation for the emitter dynamics when coupled to a general nanophotonic structure. Our framework is based on the splitting of the spectral density into two terms, leveraging the underlying physics of the light-matter interaction. On the one hand, a spectral density responsible for the non-Markovian and strong-coupling-based dynamics of the quantum emitter. On the other hand, a residual spectral density including the remaining weak-coupling terms. The former is treated nonperturbatively with a collection of lossy interacting discrete modes whose parameters are determined by a fit to the original spectral density in a frequency region encompassing the quantum emitter transition frequencies. The latter is treated perturbatively under a Markovian approximation, such that its effect is reduced to an energy shift on the emitter energy levels, which does not induce any additional numerical cost. We illustrate the power and validity of our approach through numerical calculations of the excited state population of a two-level emitter in the problem of spontaneous emission. We test three different setups supporting strong light-matter interactions: the first one is a simple model consisting of a sum of Lorentzian resonances, the second one is a realistic hybrid metallodielectric nanostructure, and the third one is a single-mode setup corresponding to a two-level emitter under ultrastrong coupling to a single physical mode.

Propagation of multisingular beams in linear and non-linear systems

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Abstract

We present a method for solving analytically the paraxial wave equation with an initial multisingular vortex Gaussian beam, that is, with a number of singularities in a plane transversal to propagation. We apply the method to study the dynamics of a quasi-two dimensional Bose-Einstein condensate (BEC) which initially contains several vortices at arbitrary locations. We study three cases: (i) homogeneous medium [1]; (ii) in a parabolic trap (which in photonics would be a Graded Index (GRIN) material [2]); and in a rotating parabolic trap. The method allows one to obtain algebraic equations for the trajectories of the position of phase singularities present in the initial condition along with time (the vortex lines). With these equations, one can predict quantities of interest, such as the time at which a vortex and an antivortex contained in the initial condensate will merge. We compare these linear (non-interacting) solutions with numerical simulations in the non-linear case (Kerr non-linearity or self-repulsive BEC) in all three cases to determine how these quantities change in the nonlinear case.

- [1] Ferrando, A., & García-March, M. A. (2016). Analytical solution for multi-singular vortex Gaussian beams: the mathematical theory of scattering modes. *Journal of Optics*, 18(6), 064006.
- [2] De María-García, S., Ferrando, A., Conejero, J. A., De Córdoba, P. F., & García-March, M. Á. (2023). A method for the dynamics of vortices in a Bose-Einstein condensate: analytical equations of the trajectories of phase singularities. *Condensed Matter*, 8(1), 12.

Artificial intelligence applied to the simulation of macroscopic high harmonic generation

1st author

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Abstract

In recent years, artificial intelligence (AI) has been proven to be a powerful tool in multiple areas of knowledge, including physics, due to its ability to detect correlations between variables. In this work we apply AI to simulate one of the most exciting strong field processes, high-order harmonic generation (HHG). HHG is computationally demanding as it requires both a microscopic description, that takes place at the sub-nanometer/attosecond spatiotemporal scales, and a macroscopic one, at the millimeter/femtosecond scales. At the electronic level, the exact description requires the computation of the laser-driven electronic wavepacket dynamics given by the three-dimensional time-dependent Schrödinger equation (3D-TDSE), whereas the full macroscopic description involves the Maxwell equations to account for propagation. However, such simulations are beyond the state-of-the-art computational capabilities, and approximations are required. In our work we demonstrate that AI can accurately reproduce the 3D-TDSE microscopic HHG response. After its coupling with the exact solution of the integral Maxwell equations, the full HHG response can be reproduced [1]. This method is especially suited to compute macroscopic HHG driven by structured laser beams carrying orbital angular momentum within minutes. In addition, it has the potential to reveal hidden signatures in the attosecond pulse emission that are neglected in the standard approximations. Our work introduces an alternative and fast path to accurately compute extreme-ultraviolet/x-ray attosecond pulse generation while preserving the quantum description given by the 3D-TDSE.

- [1] J. M. Pablos-Marín, J. Serrano, C. Hernández-García, "Simulating macroscopic high-order harmonic generation driven by structured laser beams using artificial intelligence" *Computer Physics Communications* 291, 108823 (2023)

Ultrafast sources in the UV and XUV for time-resolved spectroscopy

1st author

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Abstract

Photo-induced chemical reactions are at the basis of many biologically and chemically fundamental functions. Time-resolved photoelectron spectroscopy combining ultrashort UV and XUV pulses offers the right tools to investigate non-adiabatic dynamics, which typically evolve on ultrafast timescales (10-100 fs). In this talk, I will introduce our recently developed beamlines for investigating excited-state dynamics in organic compounds with temporal resolution ranging from sub-20 fs down to few-femtosecond. In a first scheme broadband UV pump pulses are generated by exploiting a scheme based on sum-frequency mixing and combined with tunable XUV probe pulses obtained by high-order harmonic generation. We can follow

with unprecedented detail the non-adiabatic relaxation of a prototypical molecule, acetylacetone. The extreme temporal resolution allows us to resolve for the first time the ultrashort lifetime of the S2 state and to detect the coherent modulation of the signal characterizing the first hundreds of femtoseconds of the dynamics. To further extend these methods to the attosecond time scale, few-cycle UV pump pulses obtained by dispersive wave emission in hollow-core capillaries, are directly characterized for the first time with an all-in-vacuum self-diffraction FROG and combined with single attosecond pulses. This source will be readily exploited for photoelectron/ion spectroscopy with unprecedented temporal resolution

1D and 3D Maxwell-Bloch modelling of lasing from nitrogen plasma filaments

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Abstract

Cavity-free nitrogen lasing from atmospheric plasma filaments holds the promise of delivering an intense, coherent, and directional signal, from the atmosphere towards the Earth's surface, that will improve the signal-to-noise ratio and sensitivity of LIDAR techniques using this signal. An intense IR pulse creates a plasma filament in the atmosphere that emits and amplifies radiation towards the celestial vault (forward direction) and Earth's surface (backward direction). Is this latter beam the one that is useful for LIDAR applications. In order to develop and improve this source it is necessary to fully comprehend the mechanisms behind the emission and amplification of UV radiation from N₂ ($\lambda = 337$ nm) and N₂⁺ ($\lambda = 391$ nm). When the IR pulse that creates the filament is circularly polarized, the electrons of the plasma have enough energy to, via collisional excitation, create a population inversion between the C₃^u and B₃^g vibrational levels of neutral nitrogen molecules [DanyloPRL19]. In the case of ionized nitrogen molecules, it is believed that long-lived coherences couple different levels of the molecule resulting in lasing without population inversion [MysyrowiczAPL19]. Here, we will show recent modelling results, using our 1D and 3D Maxwell-Bloch codes DeepOne [OlivaPRA11] and Dagon [OlivaSPIE17], concerning the amplification mechanism in N₂ [LopezOE23] and N₂⁺ [MeiAPS23]. We will show that the similarities with plasma-based seeded soft X-ray lasers allows to transpose well known techniques of this field onto nitrogen lasing, allowing the optimization of these amplifiers.

[1] Danylo, et al, Phys. Rev. Lett. 123, 243203 (2019)

[2] Mysyrowicz, et al, APL Photon. 4, 110807 (2019)

[3] Oliva, et al, Phys. Rev. A, 84, 013811 (2011)

[4] Oliva, et al, Proc. of SPIE, 10243, 1024303 (2019)

[5] Lopez, et al, Opt. Exp. 31, 5, 8479 (2023)

[6] Mei, et al, Acta Photonica Sinica, 52, 4, 0414001 (2023)

Passive Modelocking of Solid-State Lasers: Master Equation, Self-Starting Modelocking, and the Q-Switching Instability

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Abstract

For nearly half a century since Herman A. Haus introduced the Master Equation (ME) approach, achieving a dynamical theory of passive modelocking has remained a formidable challenge. In this work, we present a novel ME that effectively addresses the longstanding obstacles encountered, particularly concerning the presence of multiple relevant time scales governing gain and absorption dynamics. The presented ME is universally valid, applying to all types of lasers modelocked by slow or fast absorbers, featuring short or long cavities, and operating at any pumping level. Focusing on solid-state lasers, we utilize this universal ME framework to conduct a comprehensive examination of phenomena previously treated only approximately. In particular, we identify the general conditions under which modelocked pulses emerge ---the so-called self-starting modelocking (SSML) boundary in parameter space--- and explore the associated Q-switching instability, responsible for the periodic modulation of the pulse train peak intensity with a typical period embracing many cavity roundtrips. Notably, we elucidate that the SSML also dictates the transition between harmonic modelocking regimes of varying orders, characterized by pronounced hysteresis phenomena in agreement with experimental observations. Our findings contribute significantly to advancing the understanding of passive modelocking dynamics and offer valuable insights into the behavior of solid-state lasers, paving the way for enhanced control and optimization of laser systems.

Tavis-Cummings model for frequency up-conversion in gas-filled anti-resonant hollow-core fibers

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Abstract

The development of quantum transduction strategies is essential for quantum communication networks in order to be able to interconnect devices working at different optical frequencies. In this regard, broadband-guiding anti-resonant hollow-core fibres filled with molecular gases constitute a powerful tool for thresholdless frequency translation, enabling ultrahigh conversion efficiencies along with large and tunable frequency shifts. Remarkably, correlation-preserving frequency up-conversion of single photons belonging to an entangled pair was recently demonstrated in hydrogen-filled anti-resonant fibres. This was achieved by exploiting the optical phonons generated in the gaseous core via stimulated Raman scattering. Such vibrational molecular coherence prepared along the fibre length, is then used to convert the frequency of an incoming single photon with almost unity efficiency, provided specific phase-matching conditions between the generated coherence waves and the corresponding transitions are fulfilled. In addition, non-classical correlations present in the original biphoton pair were found to be preserved during the frequency translation process. It turns out that, despite its experimental evidence and robustness, this observation cannot be explained under the usual semi-classical framework based on Maxwell-Bloch equations. This is

because of the classical treatment of the optical fields, which precludes the analysis of the influence of fibre-based Raman frequency conversion on the intrinsic quantum properties of non-classical light states.

In this work, we introduce an effective N-molecule Tavis-Cummings model capable of providing a full quantum-mechanical description of frequency conversion processes occurring inside gas-filled anti-resonant fibres. In particular, this theoretical framework allows us to gain insight into the dynamics of quantum light-quantum matter interactions, predicting e.g. the preservation of entanglement under specific conditions. This tool will enable the design and optimization of future experiments aimed tailoring the properties of quantum light with unprecedented control.

Scaling of Raman molecular modulation in hollow anti-resonant fibers

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Abstract

Common optical systems where the polarization induced in the medium depends linearly on the applied field are naturally scalable due to the independence of Maxwell's equations on the optical signal strength. However, when high intensities are applied, the optical response of the medium becomes nonlinear and small changes in the light intensity yield very different outcomes, which makes it difficult to find simple scaling rules based on the properties of the governing equations. Nonetheless, it was recently demonstrated that specific combinations of physical parameters such as light intensity, beam size and propagation distance enable the scaling of highly nonlinear phenomena such as filamentation and high-harmonic generation. On the other hand, gas-filled hollow anti-resonant fibers are excellent platforms to observe such scaling owing to the exquisite control they offer over the various parameters affecting nonlinear propagation of intense optical pulses, as recently shown in the context of soliton self-compression.

In this work, we will discuss in detail the physics of stimulated Raman scattering and molecular modulation in anti-resonant fibers filled with Raman active gases and extract the key components that permit a non-trivial scaling. In particular, we have found that the complex dynamics within the fiber can be accurately reproduced in very different parametric regimes by controlling the ratio between the effective gain and dephasing lengths, as well as the overall dephasing among the interacting fields. As a result, this method enables the design of similar Raman conversion landscapes with very different pressures and fiber core diameters without sacrificing performance. Our results open up new routes to the efficient design and optimization of fiber-based nonlinear devices such as compact light sources operating in exotic frequency domains like the ultraviolet or quantum frequency converters of non-classical states such as entangled photon pairs.

Low dimensional perovskites for quantum optics and QED platforms

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Abstract

Metal halide perovskites (MHPs) have become attractive materials for light-matter interaction, and particularly for quantum optic devices [1]. Their advantages include straightforward fabrication by chemical synthesis, a broad bandgap tunability with the composition, the high emission efficiencies, and the high excitonic binding energy. Consequently, low dimensional MHPs have been incorporated in different microcavities resonators to demonstrate lasing, and more recently polariton condensation in cavity coupled lattices [1]. In this direction, perovskites 0D nanocrystals (NCs) and two-dimensional (2D) perovskites have emerged as a low dimensional MHPs with excellent properties to study Jaynes–Cummings or dressed Boson Hamiltonians. In contrast to 3D perovskites, the semiconducting inorganic layer in 2D perovskites passivated with insulating long organic cations forming a 2D quantum well structure owning a higher defect tolerance and resistance against environmental conditions [3]. Here, it will be summarized recent results from the optical characterization of low dimensional MHPs, for low-cost single photon emitters, with 0D perovskites NCs, and for high tunability QED approaches, with 2D perovskites and fibre-based open-access optical microcavities. The open-cavity approach results as an outstanding scheme to implement future disruptive semiconductor devices, which are promising candidates for the development of the exciting field of quantum polaritonics [4].

[1] M. Esmann, S. C. Wein, C. Antón-Solanas, Solid-State Single-Photon Sources: Recent Advances for Novel Quantum Materials. *Adv. Funct. Mater.* 2024, 2315936.

[2] Su, R., Ghosh, S., Wang, J. et al. Observation of exciton polariton condensation in a perovskite lattice at room temperature. *Nat. Phys.* 16, 301–306 (2020)

[3] Setatira Gorji *et al.* Origin of discrete donor–acceptor pair transitions in 2D Ruddlesden–Popper perovskites. *Appl. Phys. Rev.* 1 June 2024; 11 (2): 021401

[4] Muñoz-Matutano, G., Wood, A., Johnsson, M. et al. Emergence of quantum correlations from interacting fibre-cavity polaritons. *Nature Mater* 18, 213–218 (2019) & Delteil, A., Fink, T., Schade, A. et al. Towards polariton blockade of confined exciton–polaritons. *Nature Mater* 18, 219–222 (2019)

Enhanced emission of single-photon sources based on colloidal quantum dots with printed microstructures

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Abstract

Single-photon emitters are at the cornerstone of most quantum communication technologies. Among existing single-photon sources (SPS), core-shell colloidal quantum dots (QDs) are particularly attractive given their small size, on-demand photon production capability, and wavelength tunability within the visible range. The QDs have an isotropic emission, limiting the coupling of the emitted photons into the optical system of interest. The goal of this project is to address these issues and develop highly efficient SPS based on QDs for future integration into quantum communication systems. Our approach is based on fabricating a resonant cavity, such as a Bragg resonator, around individual QDs by using a nanoprinter with a spatial resolution of 200 nm. This not only enhances emission rates and the Purcell effect but also reduces

off-resonant emissions. Additionally, using the same nanoprinter, we can generate 3D micro-optics that improve both, the directionality of the emitted photons, as well as their quantum efficiency and stability. Here, we show our initial results on the characterization of the morphological and optical properties of individual QDs spread on top of a substrate. The latter is achieved by using a Hanbury Brown and Twiss optical system capable of measuring their antibunching behaviour. We also compare the emission characteristics with and without resonant cavities, which are in good agreement with finite difference time domain simulations. To ease the isolation and localization of individual QDs - key for the proper performance of the resonant microstructures - we are currently working on the fabrication of polymeric arrays where QDs can be anchored. Our results show promise toward the development of controlled and enhanced SPS at targeted positions on a substrate.

Finite transition quantum effects in temporal metamaterials

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Abstract

In recent years, there has been a revolutionary transformation in controlling electromagnetic waves, thanks to the emergence of time-varying media. This development has sparked theoretical investigations into new quantum optical phenomena, paving the way for groundbreaking studies. These include directional amplification of vacuum fluctuations using anisotropic temporal boundaries, ultra-fast quantum state frequency shifting with antireflection temporal coatings, innovative amplification methods, modified quantum behaviors in two-level systems, and spontaneous photon generation with time-varying gratings. What ties these efforts together is the fundamental concept of a temporal metamaterial: the temporal boundary. This boundary acts as a theoretically instantaneous switch in optical properties, or a periodic assembly of such instances. However, practical implementations unavoidably introduce finite transition times, which are expected to affect both scattering and photon production effects, and whose classical response has been studied recently under the name of tapered photonic switching.

In this study, we address the quantum phenomena of vacuum amplification effects in time-varying media with arbitrary time-modulation profiles. To understand this, we introduce the conceptual picture of conjugated oscillators to evaluate the impact of transition times at temporal boundaries, offering practical insights into observing quantum effects. Our findings intuitively reveal that faster temporal tapering results in greater photon production from quantum vacuum amplification effects. Interestingly, transition times, albeit smaller but on the same order of magnitude than the period, effectively simulate the expected behavior of temporal metamaterials simulated with a temporal boundary. Furthermore, our research extends to non-trivial effects in pulsed modulations that maximize photon production. Surprisingly, we discover that the fastest and strongest pulsed dielectric modulation does not lead to the highest photon production, providing important considerations for enhancing quantum phenomena.

Inelastic confinement-induced resonances in multiwell potentials

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Abstract

The anharmonicity that is almost always present in any optical potential that traps an ultracold gas is responsible for the coupling between the center of mass and the relative motion, which can yield inelastic confinement-induced resonances. These resonances can be used to synthesize molecular states, and may also yield losses in experiments under certain circumstances. After the observation of these resonances in quasi-one- [1] and quasi-two-dimensional [2] geometries, and under mixed dimensional setups [3], their existence under strong three-dimensional confinement has been recently shown [4]. In this communication, we report on the quantum simulator of lithium-7 atoms in an optical lattice considered by Y. K. Lee, H. Lin, and W. Ketterle [5], where the Heisenberg spin dynamics near a Feshbach resonance is studied. By considering a multiwell description of the optical trap, based only on the experimental properties of the external lasers, we show that the positions of the resonant features that are experimentally observed are in excellent agreement with the positions of the lowest-lying inelastic confinement-induced resonances with no further fittings or arbitrary adjustments [6], as in Ref. [5]. The anharmonic effects of the potential, in particular the multiwell effects, and the different symmetries of the states involved in the previous resonances will be discussed in detail.

[1] E. Haller et al., Phys. Rev. Lett. 104, 153203 (2010).

[2] B. Fröhlich et al., Phys. Rev. Lett. 106, 105301 (2011).

[3] G. Lamporesi et al., Phys. Rev. Lett. 104, 153202 (2010).

[4] Deborah Capecchi et al., Phys. Rev. Lett. 131, 213002 (2023)

[5] Yoo Kyung Lee, Hanzhen Lin, and Wolfgang Ketterle, Phys. Rev. Lett. 131, 213001 (2023).

[6] Fabio Revuelta, and Alejandro Saenz, "Inelastic confinement-induced resonances in multiwell potentials" (in preparation).

Two-photon emission from single-photon sources

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Abstract

The most fundamental source of quantum light is, without any doubt, the two-level system (2LS). Since it cannot hold more than one excitation, it always produces perfectly antibunched light, thus qualifying as the most straightforward realisation of a single-photon source. Even when considering more complex structures, such a basic picture provides further opportunities along similar lines [1]. Under weak coherent excitation, the antibunching of a 2LS is a consequence of the interference between the coherent (mean field) and incoherent (fluctuations) fractions of the emission [2]. Suppressing the former through homodyning shows that the fluctuations are strongly correlated [3], which reveals the multiphoton structure hidden behind the resonance fluorescence. This has been recently confirmed experimentally by various and complementary approaches, partially suppressing either the incoherent [4] or the coherent [5] photons through frequency filtering. When the laser-emitter detuning is large, the spectrum consists of two symmetric sidebands around the Rayleigh peak. Using frequency filtering [6], we can correlate the signal from these peaks and show that two photons, one from each band, are emitted in a cascade [7]. Additionally, the quality of the process considerably improves when the Rayleigh peak is subtracted using homodyning.

- [1] Sbresny et al., Phys. Rev. Lett. 128, 093603 (2022).
- [2] Zubizarreta Casalengua et al., Laser Photonics Rev. 1900279 (2020).
- [3] Zubizarreta Casalengua et al., Phys. Rev. A 101, 063824 (2020).
- [4] Hanschke et al., Phys. Rev. Lett. 125, 170402 (2020).
- [5] Masters et al., Nat. Photon. (2023). In press. 10.1038/s41566-023-01260-7
- [6] del Valle et al., Phys. Rev. Lett. 109, 183601 (2012).
- [7] Zubizarreta Casalengua et al., Phys. Scr. 98, 055104 (2023).

Non-linear-enabled localization in driven-dissipative photonic lattices

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Abstract

Spatial photon localization holds great significance for the control of light-matter interactions, showcasing fundamental implications in quantum information, communication, and simulation. A recent experimental work [1] has shown how driving lossy photonic lattices with multiple, spatially separated, laser spots can produce localization with dynamically tunable spatial dependence. However, an important drawback of this method is that it only works for specific combinations of laser frequencies and/or distant spots. Here, we examine this localization regime in the presence of standard optical Kerr non-linearities, such as those found in polaritonic lattices, and show that they stabilize driven-dissipative localization across frequency ranges significantly broader than those observed in the linear regime. Moreover, we demonstrate that, contrary to intuition, in most situations this driven-dissipative localization does not enhance non-linear effects like optical bistabilities, due to a concurrent reduction in overall intensities. Nevertheless, we are able to identify certain parameter regions where non-linear enhancement is achieved, corresponding to situations where emission from different spots constructively interferes [2].

- [1] O. Jamadi, B. Real, K. Sawicki, et al., Reconfigurable photon localization by coherent drive and dissipation in photonic lattices, Optica 9, 706–712 (2022).
- [2] AMH, A. Amo, and A. González-Tudela, arXiv:2401.10788 (2024).

Taming the Bloch-Redfield equation: Recovering an accurate Lindblad equation for general open quantum systems

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Abstract

Master equations play a pivotal role in investigating open quantum systems. In particular, the Bloch-Redfield equation stands out due to its relation to a concrete physical environment. However, without further approximations it does not lead to a Lindblad master equation that guarantees that the density matrix stays completely positive, which has raised some concerns regarding its use. This study builds on previous efforts to transform the Bloch-Redfield framework into a mathematically robust Lindblad equation, while fully preserving the effects that are lost within the secular approximation that is commonly used to guarantee positivity. These previous approaches introduce two potential deficiencies: the environment-induced energy shift can be non-Hermitian and some decay rates can be negative, violating the assumptions of Lindblad's theorem. Here, we propose and evaluate straightforward solutions to both

problems. Our approach offers an effective and general procedure for obtaining a Lindblad equation, derived from a concrete physical environment, while mitigating the unphysical dynamics present in the Bloch-Redfield equation.

Equilibrium parametric amplification in Raman-cavity hybrids

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Abstract

Parametric resonances and amplification have led to extraordinary photo-induced phenomena in pump-probe experiments. While these phenomena manifest themselves in out-of-equilibrium settings, here, we present the striking result of parametric amplification in equilibrium. In particular, we demonstrate that quantum and thermal fluctuations of a Raman-active mode amplifies light inside a cavity, at equilibrium, when the Raman mode frequency is twice the cavity mode frequency. This noise-driven amplification leads to the creation of an unusual parametric Raman polariton, intertwining the Raman mode with cavity squeezing fluctuations, with smoking gun signatures in Raman spectroscopy. In the resonant regime, we show the emergence of not only quantum light amplification but also localization and static shift of the Raman mode. Apart from the fundamental interest of equilibrium parametric amplification our study suggests a resonant mechanism for controlling Raman modes and thus matter properties by cavity fluctuations. We conclude by outlining how to compute the Raman-cavity coupling, and suggest possible experimental realization

Plasmonic enhancement of quantum spectroscopy for single molecule detection

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Abstract

Quantum spectroscopy methods, exploring the spectral entanglement of photon pairs, have taken a prominent role recently as a tool for absorption spectroscopy in challenging wavelength ranges like mid-infrared. Yet, due to the weakness of such single-photon level signals, extension of quantum spectroscopy and sensing methods to the level of single molecules are highly challenging. Plasmonic sensing is a powerful approach to enhance the detection efficiency of single molecules in a non-invasive way, proving to be a crucial method for various scientific disciplines, including biology and chemistry. This work explores the potential of combining plasmonic structures with a quantum spectroscopy scheme to create a sensitive method for detection of single molecules with infrared absorption lines.

We propose a scheme towards this end which explores the surface nonlinearity of a plasmonic nanoparticle. More specifically, we take a gold nanosphere, pumped around its plasmonic resonance frequency, to generate entangled photon pairs through spontaneous parametric down-conversion (SPDC). We numerically model this system using a combination of Green's function quantization methods and Mie's scattering theory.

In this scheme, the presence of a single molecule in the vicinity of the nanoparticle enhances its optical density of states at the absorption frequency of the molecule. Due to Purcell effect, this enhances the photon-pair generation rate at the molecule's absorption frequency and its paired frequency, determined by conservation of energy in SPDC. This allows the detection of the absorbing molecule by analyzing the single-photon emission rate at this paired frequency, hence offering great flexibility in the detection wavelength compared to the molecule's own absorption wavelength.

Our results demonstrate that the presence of the emitter can impact the paired single-photon rate by several orders of magnitude, and also affect its emission directionality. This shows the potential of plasmonics for pushing quantum spectroscopy methods down to a single-molecule level.

Integrating Plasmonic antennae with dielectric Waveguides towards single-molecule Raman Detection

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Abstract

In this study, we explore the functionalization of metallic surfaces using molecular monolayers, a crucial process for applications in nanophotonics and biotechnology. We present a novel approach that involves the utilization of 5-amino-2-mercaptobenzimidazole (5-A-2MBI) molecules to functionalize gold surfaces, facilitating the formation of nanoparticle-on-a-mirror (NPoM) cavities. These cavities significantly enhance light-matter interactions, enabling upconversion from terahertz (THz) to visible frequencies. The integration of NPoM cavities with silicon-based photonic chips was analytically studied. By leveraging the remarkable enhancement of Raman scattering in the near field of metallic nanoparticles and surfaces (Surface-enhanced Raman spectroscopy, SERS), the engineered surfaces enable new avenues for optimizing optical properties at the nanoscale. This integration demonstrates the potential for on-chip enhanced Raman spectroscopy and detection of infrared and THz radiation, showcasing the versatility of 5-A-2MBI monolayers across various applications. Moreover, the study explores the utilization of localized plasmonic resonances in metallic nanoparticles for single-molecule spectroscopic fingerprinting. This NPoM-on-chip integration is achieved through a combination of standard lithography and advanced nanoparticle transfer

methods. The experimental validation includes on-chip Raman detection in NPoM cavities driven by silicon nitride waveguides, showcasing the potential for advanced Raman spectroscopy.

Geometrical anticorrelations: changing the photon statistics with the geometry of the electromagnetic environment.

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Abstract

We investigate how the spatial correlations of the light emitted by two quantum emitters, modelled as two-level systems, can be totally modified by the geometry of the electromagnetic environment due to interferences between the indistinguishable optical pathways of pairs of photons. Moreover, we show how the $g(2)(r, r; \tau = 0)$ can vanish for special pairs of points, independently of the steady state of the emitters. We derive an expression for the $g(2)$ in general electromagnetic media in terms of the dyadic Green's function and we apply our theory to the next simplest case beyond the free-space: two emitters placed over a substrate. We find that the position of the zeros in the $g(2)$ can be totally different from those of the free-space, as well as the complete map of correlations. Some of these zeros are also independent of the electric permittivity of the substrate and the emitters' dipole moments. The only request is that both dipoles have to be oriented in the same direction, and the distance between them has to be larger than their natural wavelength.

POSTER: El anti-arracimamiento desde una perspectiva semiclásica

Presenter

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Abstract

Es bien sabido, desde su descubrimiento por Hanbury Brown y Twiss en los años cincuenta del pasado siglo, que la radiación clásica exhibe arracimamiento (bunching), es decir, que su grado de coherencia de segundo orden verifica $\langle g^{(2)}(0) \rangle > \langle g^{(2)}(\tau) \rangle$. La comprensión de esta propiedad, resulta casi elemental desde un punto de vista clásico. Sin embargo, desde la década de 1970 sabemos que existen estados cuánticos de la radiación que exhiben anti-arracimamiento, i.e., $\langle g^{(2)}(0) \rangle < 1$, lo que suele admitirse que requiere de la cuantización del campo electromagnético para poder ser explicado.

En este trabajo, exploramos hasta qué punto la teoría semiclásica puede explicar, al menos cualitativamente, el fenómeno del anti-arracimamiento. En primer lugar, consideramos el uso de un separador de haz (BS), de forma que se correlacionan las intensidades que llegan a sendos fotodetectores situados en los puertos de salida del BS. En este caso, el anti-arracimamiento se puede explicar por la entrada, por el puerto del BS por el que no entra la señal, de un campo semiclásico de vacío, campo compuesto por pulsos de radiación con energía menor que $\hbar\omega$. En segundo lugar, consideramos la

posibilidad de anti-arracimamiento intrínseco, que se manifiesta en la auto-correlación de la intensidad detectada por un único detector. Este anti-arracimamiento, puede explicarse semiclásicamente imponiendo la conservación de la energía, de forma que, tras cada fotodetección, la energía del haz luminoso disminuya en $\hbar\nu$ de forma adecuada. En nuestro trabajo, detallaremos el modelo de fotodetección usado, i.e., cómo cambia la intensidad del haz tras cada fotodetección, así como el resultado de simulaciones numéricas que avalan las anteriores afirmaciones.

POSTER: Scientific and technological breakthroughs in thermal emission engineering: From spatial modeling to temporal modulations

Presenter

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Co-presenter

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Abstract

The emission of thermal radiation constitutes a fundamental and universal physical process which is only attributed to the existence of a difference of temperature between two bodies. Involving thermal, optical, and quantum features, it is a multifaceted phenomenon, so that it can be approached from different perspectives. From the standpoint of thermodynamics, thermal emission is simply regarded as one of the basic mechanisms of heat transfer, with recent advances primarily concentrated on technological aspects aimed at improving the overall efficiency of thermal radiative processes, as well as the exploration of sustainable techniques for harnessing and managing thermal radiation. On a more fundamental level, thermal emission can be envisioned as a quantum process involving photon production, whose main features are enclosed within the Planck's law for the blackbody. In this realm, the most relevant progresses have been raised on the theoretical ground, particularly in the search of methods to engineer the photonic density of states, as well as the elaboration of formalisms for undertaking and unifying both thermal and quantum vacuum fluctuations. Likewise, as a radiative process, thermal emission may also be addressed from the viewpoint of electrodynamics. Upon this framework and on the basis of the Kirchhoff's radiation law, the latest advancements carried out in the field of nanophotonics have fostered the realization of artificial platforms for controlling and manipulating electromagnetic waves, thereby enabling enhanced coherence properties of thermal fields, and hence, allowing for narrowband, directive, and polarized thermal radiation, both in the far and near-field regimes. Precisely focusing on these perspectives, here we survey some of the most significant scientific and technological breakthroughs in thermal emission engineering, from fundamental aspects, new phenomena, to innovative applications, highlighting the enticing opportunities brought about by transiting from approaches based on spatial modeling to the recent proposal of temporal metamaterials.

POSTER: Evolution of pulse temporal chirp in ultralong lasers

Presenter

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Abstract

Recent years have seen the demonstration of a new family of ultralong-ultrafast fiber lasers (UUFLs) which rely on the precise management of dispersion and nonlinearities to achieve pulses in the range of hundreds

of femtoseconds and repetition rates as low as 20 kHz with no need of external compression stages. The addition of distributed Raman amplification in specific sections of the ring allows to extend the cavity length of these lasers into the tens of km while maintaining adiabatic, quasi-solitonic transmission for most of the propagation. Previous experimental measurements indicate a correlation between cavity length, chirp accumulation and key output signal characteristics such as pulse duration, that stem from deviations from ideal soliton propagation.

This work expands on this question to study how the chirp of ultrashort pulses of different shapes evolves during propagation under different amplification configurations, evaluating its potential effect on the output signal of these lasers. The proposed model uses the split-step Fourier method to simulate and study the behavior of ultrashort pulsed signals in the telecommunications C-band propagating over distances equivalent to multiple soliton periods through standard single-mode fibre, under conditions compatible with adiabatic soliton transmission.

The information generated by this model can be used to further optimize UUFL system design, getting closer to transform-limited pulse generation.

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POSTER: Stimulated Raman scattering and molecular modulation in gas-filled anti-resonant fibers

Presenter

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Abstract

Anti-resonant-reflecting hollow-core photonic crystal fibers have arisen as a disruptive technology for nonlinear optics over the last decade. This is because of their ultralow-loss broadband guidance and resilience to photo-induced damage, which have in turn lowered the threshold for the onset of nonlinear phenomena in gases by several orders of magnitude as compared to free-space arrangements. In addition, gas-filled fibers exhibit a pressure-tunable dispersion landscape that allows for additional control over strong light-matter interactions along the fiber length. Furthermore, when filled with molecular gases, roto-vibrational transitions can be efficiently excited in the fiber core via two-photon inelastic scattering phenomena such as stimulated Raman scattering. This process triggers the generation of coherence waves of synchronous molecular motion, which can then be subsequently used for efficient frequency conversion of pump pulses under many different conditions. Such molecular modulation of arbitrary fields has thus facilitated remarkable achievements ranging from the conception of efficient gas-based fiber lasers in hardly-accessible spectral ranges to nonlinear multidimensional converters or new quantum technologies.

Here we revisit the state-of-the-art applications of stimulated Raman scattering and molecular modulation in gas-filled anti-resonant fibers. Among other fields, these include development of mid-infrared and ultraviolet light sources, multi-octave-spanning Raman combs, soliton-compression schemes, or efficient quantum frequency translation approaches in the single-photon limit. We will outline the current and future trends in the field, along with an optimistic perspective to what lies ahead.

POSTER: Floquet theory in the context of nonlinear optics for isolated and extended systems

Presenter

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Abstract

Recent theoretical studies have revealed the importance of investigating higher order nonlinear response effects in models, cold atom systems, and real materials [1]. For example, the third order jerk current has been proved to be the lead generator of the dc photocurrent generated by linearly polarized light in the type-II Weyl semimetal TaIrTe₄ [2]. Here, we present a method, based on Floquet theory, to systematically treat higher order optical processes. Our approach extends beyond traditional nonlinear response theory by providing a comprehensive framework for analyzing multiphoton resonances and higher harmonic generation. By calculating the quasienergy spectrum, we offer insights into the nonlinear optical response of real materials, cold atom systems, and models, accommodating variable strength and frequency of the driving laser field. Our proposed method diverges from conventional approaches by emphasizing non-perturbative analysis of effective, time-averaged dynamics. This alternative yet meaningful methodology offers a new perspective on studying nonlinear optical phenomena, enriching our understanding of light-matter interaction in complex material systems.

[1] J. D. Pritchard, K. J. Weatherill, and C. S. Adams, "NONLINEAR OPTICS USING COLD RYDBERG ATOMS," in Annual Review of Cold Atoms and Molecules, vol. 1, WORLD SCIENTIFIC, 2013, pp. 301–350. doi: 10.1142/9789814440400_0008.

[2] Á. R. Puente-Uriona, S. S. Tsirkin, I. Souza, and J. Ibañez-Azpiroz, "Ab initio study of the nonlinear optical properties and dc photocurrent of the Weyl semimetal TaIrTe₄," Phys. Rev. B, vol. 107, no. 20, p. 205204, May 2023, doi: 10.1103/PhysRevB.107.205204.

POSTER: Solitones espaciotemporales en redes de Bessel

Presenter

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Abstract

Se presentan soluciones numéricas de solitones espaciotemporales (3+1 dimensiones) en un medio de dispersión anómala y respuesta Kerr focalizante y que presenta una distribución de índice radialmente simétrica dada por una función de Bessel de orden cero (red de Bessel). Se analizan las familias de estados estacionarios para el caso guiante, en el que la red presenta un máximo principal en el origen, así como el caso anti-guiante, en el que la red presenta un mínimo. Se analizan en cada caso tanto los estados fundamentales así como los vórtices de primer orden. Se recuperan los resultados ya conocidos para el caso de los solitones fundamentales en el caso guiante. En el caso de los estados fundamentales en el sistema anti-guiante, así como para los vórtices en ambos casos se han encontrado fenómenos de multiestabilidad (diferentes soluciones para un mismo valor de la constante de propagación). Se estudia la estabilidad de las diferentes soluciones encontrando zonas en las que dichas soluciones son estables, otras en las que hay (caso de vórtices) inestabilidad acimutal y otras en las que se produce inestabilidad de colapso.

POSTER: Spatio-Temporal characterization in VEGA-3 PW-class laser

Presenter

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Abstract

High power ultrashort pulsed lasers are used on a daily basis to accelerate particles and to study some fundamental physics as laboratory astronomy, fusion experiments, or limits of theoretical physics. For such experiments where peak power is critical, the energy, focusability, and temporal management is decisive. In those lasers, temporal and spatial characterisation is usually performed assuming an independent character, but this is not sufficient for fine corrections and leads to an appreciable reduction of peak power in focus. Measurement and control of spatio-temporal couplings is, thus, critical to ensure the proper management of the pulse. Several techniques to fully characterise the electric field have been proposed in the last decade but none of them has arisen as standard and each of them has its highlights and drawbacks.

In this contribution we present the application of a recently reported spatio-temporal technique based on the Bulk Lateral SHearing Interferometry (BLASHI), developed in the Aplicaciones del Láser y Fotónica (ALF) group of the University of Salamanca, to the characterisation of VEGA-3, the 1 PW, 1 Hz laser line at the Spanish Pulsed Laser Centre (CLPU). This technique relies on a walk-off uniaxial crystal to create two interfering beam replicas, so it presents an inline, compact, and ultra-stable setup. Preliminary results are presented, showing a spatio-spectral dependence across the pulse aperture, and technical difficulties to perform spatio-temporal measurements in PW class laser are addressed.

POSTER: Towards ultrasensitive phase-shift metrology with nonlinear optical transient detection

Presenter

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Abstract

Detecting gravitational waves and advancing precision manufacturing both demand highly accurate length and dimensional measurements, often on the nanometer scale and below. Optical interferometry serves as a go-to method for such tasks. While conventional interferometers offer uniform sensitivity across measurement ranges, there are scenarios where amplified sensitivity around specific phases proves advantageous, even if it entails reduced sensitivity elsewhere. This can be accomplished with double interferometers. Conventional interferometry derives phase from intensity measurements, limiting precision. Alternatively, we've developed an ultra-sensitive measurement system employing time-holography on outputs from two distinct yet related systems: a conventional Mach-Zehnder interferometer (MZ) and two-wave mixing in a photorefractive nonlinear crystal (PR). Time-holography, akin to traditional holography but with a frequency-shifted reference, is generated via electro-optic modulation. The temporal hologram directly accesses the phase of the complex light field through digital Fourier reconstruction, vastly enhancing sensitivity. Our system configures one MZ/PR output to a minimum (dark port), controlled by the intensity ratio of interfering beams—a key parameter. Once at this minimum, we systematically adjust the relative phase between beams (signal phase) and measure it via the temporal hologram. We've demonstrated a quasi-linear relationship between measured and signal phases, significantly amplified by factors reaching thousands. Amplification levels are controlled by the intensity ratio, with close-to-1-ratios yielding greater magnification factors—allowing detection of minute phase changes well below the nanometer level. In essence, our technique empowers precision measurement capabilities, unlocking unprecedented sensitivity for scientific and industrial applications.

POSTER: Modelling ultrafast studies from molecules to 2D materials

Presenter

Antonio Picon Universidad Autónoma de Madrid

Abstract

Novel laser sources, both based on the non-linear process of high-harmonic generation (HHG) and free-electron lasers, enables to produce pulses as short of hundreds of attoseconds ($\text{as} = 10^{-18} \text{ s}$), the natural time scale of electron dynamics. This technology unlocked an unexplored landscape of investigating electron correlations. In these studies, it is essential to also develop theoretical and numerical approaches to describe the observables. In this work we show some of the ongoing works in our group, from molecular systems to 2D materials.

Quantum Technologies Symposium (GEOCONL, GEIC) / *Simposio de Tecnologías Cuánticas (GEOCONL, GEIC)*

Organiser

Miguel Angel García March

Invited speakers

Rodrigo Martínez (DIPC- Donostia International Physics Center) Daniel Barredo (Institut d'Optique-CNRS & CINN-CSIC)

Symposium abstract

The symposium is jointly organized by the Quantum Optics and Nonlinear Optics Group (GEOCONL) and the Quantum Information group (GEIC) of the RSEF. Oral and poster communications will be presented. It is dedicated to developments in quantum technologies, excluding quantum computation. Modern quantum technologies include quantum simulation, quantum sensing and thermometry, quantum communications, quantum cryptography, or even quantum engines. Theoretical or experimental studies in systems typically used for these technologies, such as superconducting qubits, photonic systems, ion trapping, etc. are also welcomed, particularly when the work shows an improvement that impacts these technologies. Advances on quantum computing and theoretical quantum information are presented in a separate symposium.

List of abstracts at the symposium

Reservoir computing in quantum systems

1st author

Rodrigo Martínez Peña Donostia International Physics Center

Abstract

Reservoir computing is a machine learning paradigm that exploits dynamical systems to solve temporal tasks. This technique finds applications in fields as diverse as weather forecasting, stock market prediction, and communications. Similar to other unconventional computing paradigms inspired by the capabilities of the human brain, reservoir computing is concerned with hardware implementations that aim to overcome the challenges of digital computation. In this context, quantum reservoir computing is the case where quantum dynamical systems are used as reservoirs. In this talk, I will introduce the field and give a brief overview of state-of-the-art experimental implementations.

Development of Transition-Edge Sensors for different applications

1st author

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Abstract

Transition Edge Sensors (TESs) can be used as thermometers which use the superconducting-normal transition to sense small variations in temperature with extreme sensitivity. Coupled to adequate absorbers, they can be used as detectors for a wide range of radiation and/or particle energies with resolving power $R > 2000$ at 6 keV for instance. We report on the development of TESs based on superconducting Mo/Au bilayers, optimized for different applications including X-ray astrophysics, Dark Matter direct detection and quantum communications.

The use of Mo/Au proximity bilayers allows a fine tuning of the critical temperature, which for our devices is around 100 mK. The TES is polarized at constant voltage which leads to a negative electrothermal feedback and therefore a stable operation within the superconducting transition. The energy released in the absorber will raise the TES temperature and increase its resistance leading to a reduction in the polarization current. The TES is weakly coupled to a thermal bath which will restore the operation point with a time constant which can be tuned with proper design parameters. The variation in current is sensed with a SQUID which produces an amplified voltage signal proportional to the absorbed energy.

With X-ray Bi/Au absorbers a few micrometers thick, we have developed photon detectors for energies in the range 1-10 keV, of interest in astrophysics and material sciences (X-ray astrophysics, axion detection, synchrotron facilities). On the other hand, when coupled to a polar material, they make the sensing element of sensors for light Dark Matter searches. Finally, we have designed and simulated detectors for the visible and IR, for quantum communications applications. We use an innovative approach based on corrugating the Au surface to increase absorption efficiency. First prototypes have been fabricated and will soon be tested in a dedicated dilution refrigerator.

Single molecules as thermometers for cryogenic temperatures

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Abstract

Measuring cryogenic temperatures with high sensitivity and spatial resolution in the nanoscale is a challenging task, being portability and non-invasivity desirable qualities for the thermometers. Moreover, the characterization of thermal properties at low temperatures and in complex environments has become essential for understanding phenomena such as non-Fourier thermal transport, which have recently attracted great interest both for the challenging fundamental questions it poses [1] and for the potentially relevant technological implications in nanotechnology [2, 3]. Here, we present a portable nanothermometer based on a molecular two-level quantum system that operates in the (3–20) K temperature range, with temperatures and spatial resolutions on the order of millikelvins and micrometers, respectively. We validate the performance of this molecular thermometer by estimating the thermal conductivity of a nanopatterned silicon membrane, where we find a quadratic temperature dependence. In addition, we demonstrate two-dimensional temperature mapping via the simultaneous spectroscopy of multiple probes deposited onto such a suspended membrane. Overall, these results demonstrate the unique potential of the proposed molecular thermometer to explore thermal properties with submicron accuracy and unveil related phenomena manifested at cryogenic temperatures [4].

[1] Nature Review Physics, 3, 555 (2021)

[2] Nature, 539, 407 (2016)

[3] Nature Communication, 8, 15505 (2017)

[4] PRX Quantum, 4, 040314 (2023)

Photonic quantum metrology with variational quantum optical non-linearities

1st author

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Abstract

Photonic quantum metrology harnesses quantum states of light, such as NOON or Fock states, to measure unknown parameters beyond classical precision limits. Current protocols suffer from two severe limitations that preclude their scalability: the exponential decrease in fidelities (or probabilities) when generating states with large photon numbers due to gate errors [1, 2], and the increased sensitivity of such states to noise [3]. Here, we develop a deterministic protocol combining quantum optical non-linearities and variational quantum algorithms [4] that provides a substantial improvement on both fronts. The key idea of such hybrid algorithm is to use a classical optimizer to find the set of parameters of a parametrized quantum circuit implemented on the hardware such that it generates states maximizing the quantum Fisher information. In a second step of the algorithm, by maximizing the classical Fisher information, we also find optimal measurements. Our main result [5] is the generation of metrologically-relevant states with a small number of operations which does not depend on photon-number, resulting in exponential improvements in fidelities when gate errors are considered. On top of that, we show that such states offer a better robustness to noise compared to other states considered noise-resilient. Since our protocol harnesses interactions already appearing in state-of-the-art setups, such as cavity QED, we expect that it will lead to more scalable photonic quantum metrology in the near future.

- [1] C. Sayrin, I. Dotsenko, X. Zhou, et al., *Nature* 477, 73–77 (2011).
- [2] M. Hofheinz, H. Wang, M. Ansmann, et al., *Nature* 459, 546–549 (2009).
- [3] E. Polino, M. Valeri, N. Spagnolo, et al., *AVS Quantum Sci.* 2, 024703 (2020).
- [4] M. Cerezo, A. Arrasmith, R. Babbush, et al., *Nature Reviews Physics* 3, 625–644 (2021).
- [5] AMH, C. Tabares, J. T. Schneider, et al., arXiv:2309.09841 (2023).

Frequency-resolved purcell effect for the dissipative generation of steady-state entanglement

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Abstract

Generating, manipulating and preserving entanglement are essential tasks for the development of quantum technologies. However, the unavoidable interaction between the quantum system and its environment leads to the major obstacle of decoherence, i.e., the degradation of properties such as quantum coherence and entanglement. One strategy to overcome this problem is reservoir engineering [1,2], whereby interactions between the system and environment are designed to dissipatively stabilize a quantum state. Solid-state quantum emitters---like quantum dots, molecules or color centers---embedded in photonic structures stand out as particularly promising platforms for quantum technologies given their prospects of scalability and on-chip implementations. In this work, we present a fundamental mechanism for generating stationary states of nearly maximal entanglement among nonidentical interacting quantum emitters placed inside a cavity in a driven dissipative setting. Via a frequency-resolved Purcell effect, the cavity serves to amplify the transition from the highest excited state of the system to an entangled state, in which a single de-excitation is shared coherently among all the emitters. This phenomenon occurs when the emitters interact coherently, resulting in hybridized states, and the linewidth of the cavity is sufficiently narrow to distinguish the internal energy structure of the excitonic eigenstates. This allows us for resonant enhancement of the desired transition through frequency tuning. We show that this mechanism can be implemented using both coherent drive, specifically for the case of two emitters [3], and incoherent drive for any number of emitters [4]---resulting in a totally scalable mechanism of entanglement generation in the presence of dissipation [5]---. We also show that the stabilization of entanglement translates into particular features in the classical and quantum optical properties of the light emitted by the system at frequencies that are perfectly resolved, allowing to isolate the optical signatures of entanglement by simple spectral filtering.

- [1] A. Gonzalez-Tudela et al., *Physical Review Letters* 106, 020501 (2011).
- [2] D. E. Chang, et al., *Reviews of Modern Physics* 90, 031002 (2018).
- [3] A. Vivas-Viaña, D. Martín-Cano, and C. Sánchez Muñoz, Arxiv 2306.06028.
- [4] A. Vivas-Viaña, D. Martín-Cano, and C. Sánchez Muñoz, Arxiv 2312.12372 (accepted in PRL).
- [5] Häffner, H et al., *Nature* 438, 643–646 (2005).

Simple and self-testing quantum random number generator

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Abstract

Quantum random number generators (QRNGs) have obtained notable attention and undergone substantial development, driven by their utility across diverse fields including simulations, gambling, and cryptography. This surge in interest stems from their unique capacity to deliver inherent randomness, which can only be derived from the probabilistic nature of quantum mechanics. The key challenge lies in validating the quantum origin of the randomness produced, which usually requires either a thorough characterization of the elements in the setup or very experimentally challenging loophole-free bell tests. In this work, we present a simple, self-testing and cost-effective quantum random number generator (QRNG) designed to operate with an untrusted measurement device and a partially characterized source, yielding a high rate of random bits. We consider a prepare-and-measure scenario where the preparation device takes a binary input x and a binary output b is received from the measurement device. Depending on the input, the preparation device sends either a weak coherent state ($x=1$) or a vacuum state ($x=0$). The measurement device employs homodyne detection to distinguish between these states, and the output value is chosen when the detector current is below ($b=0$) or above ($b=1$) a certain threshold. In order to certify the quantum origin of the randomness generated by output b , we need to track the correlations between input and output and the average energy per pulse must respect an upper bound. By using a continuous wave laser to seed the pulsed laser that generates the states, we avoid the need for expensive electro-optical modulators as used in <https://arxiv.org/abs/2004.08307>. With this scheme we achieve an extraction rate of certified quantum randomness of around 625kHz.

A security framework for quantum key distribution implementations

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Abstract

Quantum key distribution (QKD) can theoretically achieve the Holy Grail of cryptography, information-theoretic security against eavesdropping. However, in practice, discrepancies between the mathematical models assumed in security proofs and the actual functioning of the devices used in implementations prevent it from reaching this goal. Device-independent QKD is not a satisfactory solution to this problem, as its performance with current technology is extremely poor and it cannot incorporate information leakage from the user devices without breaking the device independence assumption. On the other hand, measurement-device-independent (MDI) QKD can guarantee security with arbitrarily flawed receivers while achieving high performance, and the remaining challenge is ensuring its security in the presence of source imperfections. So far, all efforts in this regard have come at a price; some proofs are suitable only for particular source imperfections, while others severely compromise the system's performance, i.e., its communication speed and distance. Here, we solve this crucial problem by presenting a security proof in the finite-key regime against general attacks that is robust to all practical source imperfections while maintaining high performance. Moreover, our proof requires minimal state characterization, which

facilitates its application to real-life implementations. We anticipate that, thanks to these advantages, it will serve as a basis for the standardization of QKD sources.

Quantum key distribution with full information leakage

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Abstract

Quantum key distribution (QKD) enables secure transmission of cryptographic keys over insecure channels, ensuring information-theoretic security. Its distinct advantages make it a promising solution for long-term secure communications. While great progress has been made in theory and practice, several challenges remain, particularly in addressing imperfections in real QKD systems. Developing security proofs that accommodate these imperfections is crucial, as any disparities between theoretical models and practical implementations could compromise the security of the key. One of the most successful solutions in bridging this gap is undoubtedly decoy-state QKD, which provides a similar performance to that of single-photon sources by using practical laser sources emitting phase-randomized weak coherent pulses of different intensities. Typical security proofs of decoy-state QKD assume the ideal scenario in which the QKD devices of the legitimate users, so-called Alice and Bob, are perfectly isolated from the environment and do not leak any unwanted information to the channel. However, achieving this condition in practice poses a significant challenge. In this work, we present a security proof for this setup that accounts for any information leakage from Alice's internal settings, including the global phases of the emitted pulses, which has been neglected in previous studies. Despite its generality, the security proof requires minimal experimental characterization of the leakage, which makes it particularly suitable for real world usage. As an example, we apply it to tackle a specific type of information leakage due to Trojan horse attacks (THA's), in which the eavesdropper (Eve) injects light into Alice's secure module to gain information about her internal settings by analyzing the back reflected photons. In this scenario, we quantitatively evaluate the effectiveness of placing an extra phase modulator to reduce the information leakage, a countermeasure often invoked in the scientific literature but never rigorously analyzed.

Quantum key distribution with unbounded pulse correlations

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Abstract

A prevalent issue in practical applications of quantum key distribution (QKD) is the emergence of correlations among the emitted signals, which usually arise due to memory effects in the modulation devices. Although recent works have proved the security of QKD in the presence of this imperfection, they rest on the premise that pulse correlations are of finite length. However, this assumption is not necessarily met in practice, since the length of these correlations could be potentially unbounded. Indeed, the first emitted pulse could be correlated with the last one, even if very faintly. Still, intuitively, there should exist a pulse separation threshold after which these correlations become so small as to be essentially negligible, rendering them inconsequential from a security standpoint. Building on this insight, we introduce a general formalism designed to extend existing security proofs to the practically relevant scenario in which pulse correlations have an unbounded length. This approach significantly enhances the applicability of these proofs and the robustness of QKD's implementation security.

Modelling and characterization of intensity correlations for quantum key distribution

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Abstract

Quantum key distribution (QKD) has raised as an attractive alternative to classical cryptography due to its security being provided by quantum mechanics rather than relying on algorithms that could potentially be broken in the future, rendering current communications insecure. The main idea is to use quantum states in order to share a common random secret key between two parties, who then use the one-time pad scheme in order to encrypt/decrypt the message. However, many of the security proofs rely on assumptions that may not agree with reality, which may cause a protocol to be vulnerable.

In the practical implementation of QKD, a big concern is the intensity correlations arising from the limited bandwidth of real devices such as intensity modulators, which causes memory effects that can leak information to a malicious party. Some attempts have been made at introducing intensity correlations into security proofs, but most of them still make assumptions that have to be checked, like a finite correlation length.

A recent security proof gets rid of this assumption, but in turn requires a measure of the correlations to an infinite order. Experimentally, this is very hard to achieve, which is why it is important to understand where correlations come from. In this context, we propose a theoretical model based on low-pass filters in order to explain intensity correlations. We also report some preliminary experimental results with the aim of characterizing them, and compare them to simulations making use of the proposed model. Finding the model to accurately represent reality would allow us to estimate the correlation strength of any order with a lower experimental demand, relying instead in simulations, thus making the practical implementation of this security proof easier to achieve.

Security of decoy-state QKD with higher-order phase correlations in gain-switched lasers

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Abstract

Quantum key distribution (QKD) protocols, leveraging quantum mechanics, hold the potential to distribute symmetric cryptographic keys that are information-theoretically secure. However, certifying the security of practical QKD implementations requires to account for experimental constraints and device imperfections. A concerning example of the latter is given by phase correlations across laser pulses in QKD schemes utilizing weak coherent laser pulses (WCPs). While these pulses are often treated as classical mixtures of photon number states assuming perfect phase randomization, this stops being the case for lasers operating under high-speed gain-switching conditions. Here, residual photons within the cavity can induce phase correlations across successive pulses, violating the prerequisite of uniformly random phases.

Recently, a security proof resilient against such imperfection has been proposed. Its application requires knowledge of a parameter quantifying the proximity of the conditional distribution of each phase to a uniform distribution, given information about all other phases. Thus, a crucial step towards guaranteeing the security of QKD implementations is determining how to experimentally estimate this parameter. Presuming a correlation length of one, the dispersion of the phase probability distribution can be estimated by measuring the visibility of interference between adjacent pulses. Nonetheless, in practical high-speed setups, significant correlations might extend beyond immediately adjacent pulses.

In this work we extend existing approaches by introducing an experimental method to characterise this parameter in the case of arbitrary length of correlations in realistic setup conditions. In particular, we focus on modeling the phase generation process inside the cavity in the presence of multiple correlating factors as an extension of known studies on first-order correlations. Moreover, we design an implementable experimental routine to enable the measurement of the required parameter for the aforementioned security proof.

A refined statistical bound for QKD security analyses

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Abstract

Security analyses of QKD require to upper bound the probability of a "failure" in the parameter estimation step of the protocol. For a variety of protocols, this task can be accomplished by invoking a suitable tail bound on the hypergeometric distribution. In this work, we propose a simple alternative that exploits an elementary link between hypergeometric and binomial random variables. Despite the simplicity of the idea, a singular improvement is obtained in the estimation of the desired bound.

Exploring quantum magnetism with Rydberg atom arrays

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Abstract

Rydberg atoms in arrays of optical tweezers offer new perspectives for quantum simulation, computation and metrology. In this talk, we will give an overview about this architecture and describe ongoing work to control Rydberg interactions to explore different types of spin Hamiltonians and generate entanglement [1]. We will present recent results on the implementation of the dipolar XY model with more than 100 spins to study quantum magnetism [2]. We will explore different magnetic orders depending on the ferromagnetic or antiferromagnetic nature of the interactions. We will illustrate how entanglement in the out-of-equilibrium dynamics of these systems can be harnessed to generate scalable spin squeezing [3]. Finally, we will see how the analysis of the spread of correlations allows us to measure the dispersion relations in the dipolar system [4].

[1] Bornet et al., arXiv:2402.11056.

[2] Chen et al., Nature 616, 691 (2023).

[3] Bornet et al., Nature 621, 728 (2023).

[4] Chen et al., arXiv:2311.11726.

Teleportation of a particle's mass via quantum Zeno dynamics

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Abstract

Teleportation in quantum mechanics usually refers to the teleportation of a quantum state through entanglement of distant particles. Instead, we report theoretically on the possibility of teleportation of a single quantum particle. Teleportation with this meaning is theoretically possible for a particle initially at rest (with a certain uncertainty) out of any equilibrium point of a potential well or barrier whose state of rest is frequently monitored. This is an example of quantum Zeno dynamics that inhibits particle acceleration, and features disappearance from the classical turning point and appearance in another, if any, with a probability that approaches unity by increasing the frequency of the measurements. This phenomenon has all the ingredients attributed in sci-fi to teleportation: The particle is always at rest, cannot be found in the path between the two turning points, and saves travel time. Indeed, we show the absence of probability flux in the path between the original location of the particle and its destination, violating the continuity equation for the probability density. We discuss the feasibility, in principle, of teleportation of electrons, protons, and heavier particles, and conclude its increasing impracticability. Nevertheless, our study establishes a basis for further research where more accurate models of measurements were to be incorporated, and relativistic equations used.

Chiral states in rotating BECs with current-density interactions

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Abstract

Persistent currents in quasi-one-dimensional Bose-Einstein condensates become chiral in the presence of current-density interactions, which emerge from an artificial gauge potential that depends on the local atomic density. This phenomenon is explored in ultracold atoms loaded in a rotating ring geometry, where diverse current-carrying stationary states are analytically found to generalize previously known solutions to the mean-field equations of motion. Their dynamical stability is tested by numerical simulations that show stable currents for states with both constant and modulated density profiles, while decaying currents appear only beyond a unidirectional velocity threshold. Recent experiments in the field place these states within experimental reach.

Simulating the 2D Fermi-Hubbard model with ultra-cold fermions in optical lattices

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Abstract

Exploring the phase diagram of the 2D Fermi-Hubbard model is an experimentally difficult task for quantum simulators, currently unable to reach low enough temperatures. There is, however, a way around this issue by virtually filtering easy-to-prepare initial states down to the desired energy window and only requiring the simulator to provide Loschmidt echoes of the said states. Herein, we explore these ideas and explain the details that have to be sorted out, such as preparing suitable initial states and computing the echo phases via short imaginary time evolution. Our proposed algorithm is best suited for being implemented in simulators that contain the Fermi statistics as a native resource, thus avoiding extra overheads derived from non-local fermion-to-qubit mappings.

Ultracold dipolar bosons trapped in a 3-well atomtronic circuit

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Abstract

The atomtronics field studies the wide set of characteristic features of quantum gases, such as entanglement, transistor-like properties and persistent currents; and capitalizes on them to develop quantum devices [1]. The typically low decoherence/dissipation rates of cold atoms systems and the high controllability and enhanced flexibility of potentials for ultracold matter make atomtronics very attractive for enlarging the scope of existing cold-atom quantum technology [2]. Triple well potentials have gained interest due to their simplicity but rich phenomenology [3,4]. Moreover, the fully connected triangular arrangement provides the smallest system to feature angular momentum and quantized vortices with a superfluid phase.

In our investigation, we analyze the behaviour of a small ensemble of dipolar bosons confined in this minimal system, with a focus on in-plane dipole orientation across multiple configurations. The system is described by an extended Bose-Hubbard Hamiltonian.

We investigate ground state properties for a wide range of on-site interaction and dipolar interaction strengths. We find that the system shows very rich phenomena as we vary the polarization angle, e.g. the entanglement between sites depends on the dipole direction. Moreover, we characterize the system studying the coherence properties and find that dipolar interactions maintain the condensed state with little depletion in the studied range of dipole strengths, which could be an advantage to sustain superfluid currents. We underscore the prospective utility of dipolar interaction as a facilitative mechanism for manipulating entanglement within the system.

[1] L. Amico, et al., AVS Quantum Sci. 3, 039201 (2021).

[2] L. Amico, et al., Rev. Mod. Phys. 94, 041001 (2022).

[3] Sudip Kumar Halder and Ofir E Alon, *J. Phys.: Conf. Ser.* 1206 012010 (2019).

[4] Karin Wittman W., et al., Phys. Rev. E 105, 034204 (2022).

Bright and dark solitons in nonlinear quantum walk

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Abstract

We propose a photonic nonlinear quantum walk model, and consider the space-time continuum limit of the evolution equation, which takes the form of a nonlinear Dirac equation. This continuum limit shows the

existence of different solitonic structures, such as bright and dark solitons, that are illustrated by numerical calculations.

On-chip time-bin entanglement at telecom wavelengths

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Abstract

Future-proof implementations for quantum communication need to be integrated on-chip, reliable, and compatible with the existing fiber infrastructure. We present a hybrid photonic integrated circuit consisting of a semiconductor photon-pair source at telecom wavelengths and a polymer interposer hosting the required passive optical elements.

The photon pairs are created in a 1.5mm long AlGaAs Bragg-reflection waveguide via parametric down-conversion. By pumping with pairs of pulses the correlated photons are born into a superposition of an early and a late time bin. The polymer interposer filters the remaining pump light reaching a 68dB suppression and then separates the photons with a >25 dB extinction ratio at a polarization beam splitter. The performance of these on-chip components is on par with their bulk counterparts.

The mechanically and optically stable coupling of photon-pair source and polymer chip as well as the fiber pigtailings suppress accidental coincidences and thereby improve the quality of the entanglement. Our state tomography confirms a 96(-8,+3)% concurrence and a 96(-5,+2) fidelity to a Bell state.

The hybrid integration method used for this photonic integrated circuit allows us to leverage the strengths of two different material platforms. The high nonlinear susceptibility of the AlGaAs is combined with the possibility of adding thin-film optical elements in the polymer interposer. The result is a photonic integrated circuit that can feed high quality time-bin entangled photon pairs into existing fiber networks.

Many-body phases enabled by quantum optical processes

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Abstract

Many-body physics and quantum optics have traditionally worked on opposite sides of the physics spectrum. Quantum optics deals with the precise quantum control of atomic, optical, and solid state systems with a small number of degrees of freedom. Many-body physics is typically associated with the statistical behavior of condensed-matter systems containing an infinite number of constituents. However, we are now in an era where our level of control of quantum-optical systems is so precise, that we can apply it to the design of devices that implement many-body models in unconventional regimes, so-called quantum simulators. So far, the main focus has been on the access to novel observables and dynamical conditions related to condensed-matter models. However, the potential of quantum simulators goes beyond the traditional scope of condensed-matter physics: Quantum simulators allow for processes such as driving and dissipation that are typically not considered in condensed-matter physics. These processes can enrich in unexplored ways the phase diagram of well-established models, as well as help stabilizing elusive phases of matter. Here we present results in both these directions. Firstly, taking the extended Bose-Hubbard model as the guiding example, we examine the impact of coherent pair injection, a process readily available in, for example, superconducting circuits. We prove that this process favors both superfluid and density-wave order, as opposed to insulation or homogeneous states, thereby providing a novel route towards the access of supersolidity. Secondly, we examine the potential of arrays of Van der Pol oscillators, paradigm for a self-sustained oscillator, to achieve time-crystalline order as a steady state. We show that while quantum fluctuations destroy phase coherence for a single oscillator, the many-body protection present in the array can bring the required robustness, depending on the dimensionality.

Setup for the complete characterization of polarizarion-entangled photons using Quantum State Tomography

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Abstract

Entanglement is one of the key features of quantum mechanics that is behind the so-called second quantum revolution [1]. Its production and subsequent characterization are of paramount importance for the development of quantum technologies. These range from secure key exchange for encryption and message encoding, to quantum teleportation of states, and a future quantum internet network. Thus, it is clearly relevant to have versatile setups where entangled photons can be produced and their entanglement can be checked, for instance by means of violating a Bell inequality. We present an experimental setup with two operation modes where entangled photons are produced by means of parametric down conversion and then are characterised by performing a full quantum state tomography and measuring the CHSH inequality. The difference between the two operation modes is that in the first one only two single photon detectors are needed while in the second one we use four detectors, thus substantially reducing the measurement time.

The idea of the setup is to be versatile in order to be able to characterise pairs of photons provenient from other sources such as solid state sources based on quantum dots. With it, one can both measure a Bell inequality or perform a tomography of the two photon state thus fully characterising their quantum state, also, as the setup was built keeping in mind the simplicity and versatility, can be also used by students at

both the undergrad and master level. Our setup has significant improvements with respect to previous works [2], notably, the quantum state tomography is performed, different Bell states can be considered and, technically, the alignment is made significantly easier.

[1] J. P. Dowling and G. J. Milburn, Quantum technology: the second quantum revolution

[2] D. Dehlinger and M. Mitchell, Entangled photon apparatus for the undergraduate laboratory

Development of a spin qubit technology platform based on semiconductor quantum dots

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Abstract

The advancement of semiconductor technologies in the field of quantum computing is experiencing significant progress. Quantum computing offers potential to carry out exponentially more efficient algorithms compared to classical computing, although they require very precise fine-tuned characteristics to mitigate de-coherence. Semiconductor devices exhibit outstanding properties as high-quality qubits, and leverage the capabilities of their established technology. This work reports the development of technological solutions for semiconductor qubits, focusing in particular on electron spins in quantum dots (QD). Two manufacturing directions are presented.

The first is based on Si nanowires (NW), where the confinement is provided in two dimensions by the NW itself, complemented by gate electrodes around the NW for further confinement along its axis. A novel fabrication strategy has been developed, consisting of mix and match of optical and electron beam lithography, where the resist is sequentially exposed in the same lithography level, followed by a common development step. This approach enables the fabrication of NWs at wafer level, taking advantage of the high-throughput of one technique while maintaining the high-resolution of the other, respectively.

The second approach consists of defining multiple gates to generate electrostatic QDs in a 2D electron gas. Two parallel gates are placed in a planar MOS channel that function as potential barriers for the QD, while a third electrode controls the energy levels of the QD. The fabrication includes the definition of field oxide, active areas, doped source/drain areas, gate oxide and three metal levels. The starting point is the in-house CMOS technology at IMB-CNM.

In summary, this work presents two distinct strategies to set-up a flexible platform for the manufacturing of QD-based devices, with special aim of exploring novel concepts for semiconductor qubits.

Satellite-based entanglement distribution and quantum teleportation with continuous variables

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Abstract

Advances in satellite quantum communications aim at reshaping the global telecommunication network by increasing the security of the transferred information. Here, we study the effects of atmospheric turbulence in continuous-variable entanglement distribution and quantum teleportation in the optical regime between a ground station and a satellite. More specifically, we study the degradation of entanglement due to various error sources in the distribution, namely, diffraction, atmospheric attenuation, turbulence, and detector inefficiency, in both downlink and uplink scenarios. As the fidelity of a quantum teleportation protocol using these distributed entangled resources is not sufficient, we include an intermediate station for either state generation, or beam refocusing, in order to reduce the effects of atmospheric turbulence and diffraction, respectively. The results show the feasibility of free-space entanglement distribution and quantum teleportation in downlink paths up to the LEO region, but also in uplink paths with the help of the intermediate station. Finally, we complete the study with microwave-optical comparison in bad weather situations, and with the study of horizontal paths in ground-to-ground and inter-satellite quantum communication.

Topological quantum dissipative phases with trapped ions

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Abstract

We simulate topological dissipative phases in a one-dimensional chain of trapped ions with their vibrational degrees of freedom. First, we study non-reciprocity in a two-ion parametric dimer and then we analyze topological amplification in larger chains where Coulomb long-range couplings become apparent. The existence of topologically non-trivial phases in this non-Hermitian system leads to the presence of edge states that produce amplification being robust against disorder. The control of the parametric driving terms is achieved by taking advantage of state-of-the-art Floquet engineering techniques. We characterize the stability of the system and find stable topological amplifiers and two-mode Gaussian steady-states that can produce entanglement.

Quantum simulators are experimental devices with controllable quantum dynamics, designed to mimic a target complex quantum system or to explore intricate quantum many-body phases. In this work, we focus on a driven-dissipative Hamiltonian model based on the phononic dynamics related to a one-dimensional chain of trapped ions.

Controlling the propagation and amplification of signals provides important advantages in different applications related to quantum technologies. On one hand, robust to disorder amplification allows the read-out of weak fields with an exponential gain while attenuating the unwanted noise. On the other hand, directionality of the signal enhances the control of the output field and reduces back scattering. Combining both features achieved by topological effects, trapped ions technologies constitute a promising candidate for processing quantum information and also a key resource for quantum sensing and metrology, going from axion Dark Matter detectors to very precise measurements in material science.

POSTER: Implementación Óptica de Paseos Cuánticos con Moduladores Espaciales de Luz

Presenter

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Abstract

Los Paseos Cuánticos (QWs: quantum walks), tanto en su versión continua como en la discreta, son una importante herramienta en información cuántica. Un QW discreto consiste en la evolución, en un espacio de posiciones, de un “caminante” que lleva asociado un qubit, de forma que su desplazamiento está condicionado por el estado del qubit. Así, en cada paso del QW, el caminante (i) se desplaza, condicionalmente, a lo largo de la red de posiciones y, seguidamente, (ii) se realiza una transformación unitaria sobre el qubit. Estas dos operaciones se repiten en cada paso de la evolución. Es bien sabido que los QWs pueden implementarse utilizando ondas clásicas; es decir, no es necesario que se trate de un sistema propiamente cuántico descrito por una función de onda. De hecho, son mayoría las implementaciones de QWs en plataformas fotónicas en las que, por ejemplo, el papel del qubit lo juega el estado de polarización de la luz, y el papel del espacio de posiciones lo juega la frecuencia del haz luminoso. En este trabajo, implementamos el QW utilizando moduladores espaciales de luz (SLM) programables. El papel del qubit lo juega el estado de polarización del haz de luz, la red de posiciones consiste en rectángulos localizados en diversos puntos del modulador, y el desplazamiento se lleva a cabo espacialmente con un prisma anisótropo, de forma que el haz es desviado a derecha o izquierda dependiendo de la polarización. La transformación unitaria, que modifica el estado de polarización en cada paso, se realiza en el propio SLM. Esta es una de las características más interesantes del montaje, pues permite poder codificar una transformación unitaria diferente en cada posición de la red bidimensional en la que ocurre el paseo cuántico. Los resultados preliminares muestran que esta es una plataforma apropiada para implementar QWs bidimensionales con control local de la transformación unitaria sobre el qubit.

POSTER: Strongly correlated few-atomic states

Presenter

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Abstract

We discuss how strongly correlated states can be obtained in systems of a few ultracold bosons belonging to different species, within current experimental capabilities. Two parameters are used to realize such states: the experimentally controllable interaction strength and the species-dependent mass ratio. We consider two distinguishable impurities immersed in a third ultracold bosonic species with an equal or

higher mass, playing the role of a bath, all confined in a one-dimensional harmonic trap. We numerically obtain the ground state of the system and show that the two impurities exhibit non-classical correlations. Our goal is to characterize them as a Bell state, mediated by the bosonic bath. Our analysis is based on measuring the correlations between the two impurities in the position basis, which is experimentally accessible. We comment on possible applications in quantum technologies.

POSTER: One and two ultracold atoms in one dimension in presence of delta potential

Presenter

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Abstract

We show that systems of one or two atoms (bosons, fermions, or distinguishable) interacting via contact delta-like interactions in presence of one or more delta potential barriers and confined in one dimensional parabolic or square well potentials offer a perfect playground to study the interplay between integrability, discrete symmetries, fragmentation of the Hilbert space, adiabaticity, and non-trivial topological phases. We study a collection of mathematically related cases where adiabatic loops on control parameters are implemented theoretically. We obtain different kinds of loops, particularly finite periodic and infinite but subjected to fragmentation ones. We discuss possible implications for their use in quantum technologies.

POSTER: Minimal thermal and thermoelectric rectifiers

Presenter

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Abstract

Modern electronic devices are currently operated at the nanoscale regime, where overheating becomes a problem. Controlling the undesired heat flows in a useful manner is another less explored way of improving its performance. For this, efficient thermal diodes need to be designed [1]. Usual proposals rely in nonlinear scenarios [2]; here, we identify the minimal conditions for a nanoscale device to rectify the heat and thermoelectric currents, even in the absence nonlinearities. This is achieved for asymmetric coherent conductors that allow for some local thermalization of the heat carriers. We quantify the amount of rectification achieved by this mechanism in some proposed systems composed of resonant-tunneling quantum dots and compare (and combine) it with the nonlinear scenarios. Finally, we propose feasible experimental realizations of this idea in an elastic conductor where the interplay between thermalization and nonlinearities can be controlled via quantum interference [3].

[1] G. Benenti et al., Springer International Publishing (Cham, Switzerland), 2016.

[2] B. Li et al., Phys. Rev. Lett., 93 (2004) 184301.

[3] R. Sánchez et al., Phys. Rev. B, 104 (2021) 115430.

POSTER: Fabrication of superconducting resonators on diamond substrates with implanted NV- centres

Presenter

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Abstract

NV- implanted on diamond are suitable candidates to store quantum information due to their long decay (T_1) and decoherence (T_2) times. The usual way to interact with them and exploit their properties is to couple the NV- ensemble within the diamond via a superconducting resonator. The coupling rate (G), which characterizes the ensemble – resonator interaction, is a crucial parameter measuring the rate at which photons are interchange between them. It is desirable a strong coupling, meaning that G is higher than the individual loss rates of both systems, to successfully transfer information from the resonator to the NV-centres. It is possible to attain a strong coupling rate using an ensemble with a high concentration of NV-centres (n), since G is proportional to the square root of n , but this increase comes with an undesired decrease in the decoherence time due to inhomogeneous broadening.

Here, we show the successful fabrication of superconducting Lumped Element Resonators (LERs) on diamond substrates with NV- centers already implanted within them. The resonators, fabricated of NbTiN, show a high internal quality factor ($> 10^5$) with a low concentration of Two-Level Systems (TLS). We have chosen LERs as a preferred design due to their properties, in particular, their small size compared to the photon wavelength, leading to a concentrated magnetic field mode volume, which mediates the coupling with the NV- centres. This strategy reduces to zero the distance between the ensemble and the resonator and allows benefitting from the mode volume region where the magnetic field is strongest.

This development opens the door to achieving strong coupling to small NV- ensembles, a desired feature to optimize the decoherence time of the system.

Didactics and History of Physics (GEDH) / Didáctica e Historia de la Física (GEDH)

Organiser

Gabriel Pinto Cañón and Luis Moreno Martínez

Invited speakers

Erramun Martiarena Sarasola

Symposium abstract

This Symposium aims to be a forum for the exchange of knowledge and discussion in which it will aim to: (i) contribute to the formation of scientific culture (especially in the field of the history of physics); (ii) share experiences and ideas of teachers from the different educational stages on the teaching of physics (educational methods, new legislation, STEM/STEAM competencies, learning situations...); (iii) promote the dissemination of science in general and physics in particular. The research areas that this symposium seeks to cover include: the didactics of experimental sciences, the history and philosophy of science, and scientific communication and dissemination.

Este Simposio pretende ser un foro de intercambio de conocimientos y discusión en el que se pretenderá: (i) contribuir a la formación de la cultura científica (especialmente en el ámbito de la historia de la física); (ii) compartir experiencias e ideas del profesorado de las distintas etapas educativas sobre la enseñanza de la física (métodos educativos, nueva legislación, competencias STEM/STEAM, situaciones de aprendizaje...); (iii) fomentar la divulgación de las ciencias en general y de la física en particular. Las áreas de investigación que trata de cubrir este simposio incluyen: la didáctica de las ciencias experimentales, la historia y filosofía de la ciencia, y la comunicación y divulgación científica.

List of abstracts at the symposium

Reflexiones y experiencias para mejorar la enseñanza de la física dentro de la educación STEAM

1st author

Erramun Martiarena Sarasola Scientix & Ikastolen Elkartea

Abstract

Invitaremos a una reflexión didáctica que guíe en la actuación docente personal, a partir de ejes fundamentales para el desarrollo de las competencias científico-tecnológicas del alumnado. Alumno-ciudadano con alfabetización científica básica.

A partir de la breve presentación de una propuesta práctica para el diagnóstico pedagógico de los centros y los departamentos didácticos, y mostrando varios ejemplos concretos, se propondrán algunas vías para profundizar tanto en la mejora organizativa como en la mejora metodológica de la práctica docente de las áreas científicas.

¿Por qué resulta útil disponer de un enfoque coordinado entre el profesorado de las áreas STEAM, para un desarrollo coherente de las competencias del alumnado? ¿Es suficiente con renovar la legislación y disponer de un buen currículum para cada asignatura y garantizar la transmisión de conocimientos?

¿Cómo podemos incidir en el ambiente del aula desde la evaluación?

¿Qué ocurre cuando el equipo directivo es sensible a la ciencia y tecnología y es capaz de liderar la cultura científica en el centro escolar?

¿Es todo cuestión de aumentar las inversiones en recursos materiales de última generación?

¿Y si acercamos a científicos-as (Físicos) reales a ese alumnado auténtico?

Este simposio tiene como objetivo compartir la experiencia profesional en el desarrollo de proyectos curriculares, el desarrollo e implementación de situaciones didácticas y proyectos didácticos STEAM, así como la formación de profesorado relativa a los mismos. Todo ello en un contexto de acompañamiento para la de Mejora Pedagógica de Centros de educación obligatoria.

Un enfoque de enseñanza activa en la Universidad: STEAM-Active

1st author

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Co-autors

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Abstract

Cada vez son más las Facultades de Ciencias y Escuelas de Ingeniería donde se aplican enfoques de enseñanza para el desarrollo de habilidades científico-técnicas. El desarrollo de este tipo de competencias en los estudiantes es un requisito para la rápida adaptación de los egresados en el mundo empresarial y tecnológico. Esto implica la necesidad de diseñar e implementar materiales de enseñanza basados en el planteamiento de proyectos STEAM cuya resolución exige el trabajo conjunto de varias disciplinas. Este enfoque transdisciplinar basado en proyectos STEAM se ha desarrollado dentro del proyecto Europeo ERASMUS+ “STEAM-Active” que se presentará en esta comunicación. El objetivo es mostrar el protocolo realizado para el diseño de materiales de enseñanza en proyectos STEAM en grados universitarios y las principales pautas para desarrollar e implementar Secuencias de Enseñanza/Aprendizaje bajo un enfoque de aprendizaje basado en proyectos. Se mostrarán ejemplos ya implementados por las diferentes universidades que participan en el proyecto STEAM-Active.

Análisis de dos enfoques de resolución de problemas de cinemática en estudiantes universitarios

1st author

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Co-author

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Abstract

En esta investigación se examinan diferentes enfoques pedagógicos utilizados para enseñar a los estudiantes cómo abordar y resolver problemas de física, específicamente en el contexto de la cinemática. Se compara la eficacia de dos estrategias: el método tradicional de resolución de problemas, que se basa en el uso indiscriminado de fórmulas, frente al enfoque de resolución de problemas basado en el uso de la derivada e integral. La investigación se llevó a cabo con estudiantes de Ingeniería Civil en la Universidad del Bío-Bío, Concepción, Chile. Los métodos considerados incluyeron el uso del vector de posición y el empleo de la derivada e integral para determinar los parámetros de cinemática. El objetivo principal de esta intervención fue proporcionar a los estudiantes un significado físico y práctico a todo el desarrollo matemático implicado en la solución de problemas, con el fin de ayudarles a comprender la física subyacente en cada situación. Estos enfoques buscan ofrecer a los estudiantes una comprensión profunda

de los conceptos, eliminando la necesidad de memorizar fórmulas generales. En su lugar, se promovió la comprensión integral de cada término dentro del vector de posición o el uso de la derivada e integral como método único para resolver problemas.

Para analizar las diferencias en las variables de estudio entre ambos grupos, se emplearon técnicas estadísticas no paramétricas. Los resultados obtenidos fueron alentadores, ya que revelaron diferencias estadísticamente significativas a favor del grupo experimental, respaldando la eficacia del enfoque adoptado. Estos hallazgos resaltan la importancia de integrar el conocimiento conceptual y matemático en la enseñanza de la cinemática para lograr un aprendizaje más profundo, estable y significativo.

Jupyter Book as a Tool for the Elaboration of Final Degree Projects in Physics and Nanothermodynamics: A Case Study

1st author

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Abstract

In the realm of scientific research and education, the effective communication of ideas and findings is paramount. In this context, the development of versatile and user-friendly tools to facilitate the creation of comprehensive documentation is of significant value. This work presents Jupyter Book (JB) as a powerful and accessible software tool for the elaboration of Final Degree Projects (TFGs) in the Degree in Physics at the UPV/EHU. Additionally, it showcases the potential of Nanothermodynamics as a complementary educational resource.

The JB emerges as a compelling platform for TFGs due to its inherent characteristics of simplicity, power, and versatility. Its user-friendly interface allows for rapid implementation, while its interactive and shareable nature fosters collaboration and dissemination of knowledge. Furthermore, JB's adaptability caters to the diverse needs of TFGs, ranging from the creation of the Memory and presentation to the preparation for the defense.

To exemplify the aforementioned capabilities, we present the electronic book Nanothermodynamics. This resource, stemming from the transformation of a TFG Memory, serves as a valuable educational tool for students in the field of Thermodynamics and Statistical Mechanics. Nanothermodynamics offers a novel perspective on finite-size effects, crucial for understanding small and finite systems.

Importantly, the use of JB and the emphasis on accessible educational resources like the Nanothermodynamics book directly align with the Sustainable Development Goal 4: Quality Education; by promoting open-source tools and freely available knowledge.

In conclusion, JB stands as a remarkable instrument for the elaboration of TFGs, providing a streamlined and effective means of documentation. Moreover, the electronic book Nanothermodynamics highlights the significance of this subfield within thermodynamics. The integration of JB and Nanothermodynamics into the educational landscape holds immense promise for enhancing the learning experience, fostering a deeper understanding of complex scientific concepts, and ultimately contributing to a more sustainable future through accessible education.

KEYWORDS: Jupyter Book, Nanothermodynamics, Thermodynamics, Statistical Mechanics, Education.

Link to Jupyter Book: <https://nanotermosp.netlify.app/intro.html#>

Educational tours through Madrid for physics learning

1st author

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Abstract

Over the past two years, we have developed educational and outreach tours in the city of Madrid, applying the educational methodology known as service-learning. This methodology aims to enhance the quality of learning, strengthen the connection between educational institutions and their surroundings, and address social needs by providing a service to the community, carried out by students.

The objectives of our work were to provide a holistic education for engineering students by connecting science, technology, art, and history; to develop their competencies (teamwork, creativity, etc.); to establish new channels for disseminating information for the Madrid City Council; to share science, art, and history with diverse audiences; and to enhance appreciation for the cultural Spain's heritage. To achieve these goals, a group of professors and students from Universidad Politécnica de Madrid designed and implemented (both on-site and through conferences) the tours "The Spanish Enlightenment and the discovery of three chemical elements" and "The 'altos del hipódromo': a landmark area of the Silver Age of Spanish culture."

In addition to detailing these tours, the methodology employed, and the results achieved, published before, we take advantage of the celebration of the XXXIX RSEF Physics Biennial to present some implications relevant to this field. For example, in the first tour, which describes the Spanish contribution to the discovery of Pt, W, and V, several aspects of interest in the history of physics in the 18th century are discussed. For instance, some contributions of Antonio de Ulloa are highlighted besides the discovery of Pt, such as geodetic measurements, observations of what are still known as "Ulloa's rings", etc. In the second tour, aspects such as the importance the Junta para Ampliación de Estudios are described, along with the work of prominent physicists (such as Blas Cabrera), and visits to Spain by Einstein and Marie Curie.

El Museo del Prado y el CERN como escenarios de aprendizaje STEAM para explorar la historia de la física

1st author

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Abstract

La educación STEAM aboga por una enseñanza que integre y relacione distintas disciplinas y ramas del saber, como ciencia, ingeniería y arte. Asimismo, la literatura académica sobre los muchos usos educativos de la historia de la ciencia ha subrayado su gran interés para humanizar la ciencia, conectando las materias de ciencias con aspectos sociales y culturales, algo que suele ser más frecuente en el caso de la enseñanza de materias del ámbito humanístico. La presente comunicación presenta dos experiencias docentes diseñadas para la materia de Física y Química de Educación Secundaria Obligatoria que incorporan tanto el

enfoque STEAM como la apuesta por el valor educativo de la historia de la ciencia. La primera experiencia (reconocida como Experiencia Educativa Inspiradora por el Ministerio de Educación, Formación Profesional y Deportes y publicada en libre acceso por el Instituto Nacional de Tecnologías Educativas y Formación del Profesorado) hace uso de parte del patrimonio artístico del Museo Nacional del Prado, disponible gracias a las TIC, para ofrecer un escenario de aprendizaje privilegiado para que el alumnado de 4º ESO reflexione sobre la naturaleza de la física como ciencia, su relación con el arte y con la sociedad, su papel en el estudio del universo o las distintas formas de producción y divulgación del conocimiento científico. La segunda experiencia ofrece un conjunto de actividades centradas en el CERN en el marco del Programa para Profesores de la Comunidad de Madrid. Las distintas actividades hacen de este centro fundamental en la investigación física actual un escenario pedagógico idóneo para abordar múltiples contenidos del currículo de las materias de Física y Química de 2º a 4º ESO (como la estructura de la materia, la energía o las fuerzas) a la par que permite introducir aspectos básicos sobre física de partículas en las aulas, área frecuentemente desatendida pese a su gran relevancia.

A software for the automated principal-component analysis of learning styles (CHAEA3S)

1st author

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Abstract

In this communication, we present CHAEA3S, a software package designed for comprehensive analysis of learning styles within classroom environments. CHAEA3S can be applied to elementary, secondary and high educational levels. The developed software implements the automatic analysis of the Honey-Alonso questionnaire, which categorizes students into four different categories: activist, theorist, reflector, and pragmatist. CHAEA3S is user-friendly and accessible, requiring no prior programming expertise, thereby enabling educators to effortlessly gain insights into the learning preferences of arbitrary numbers of students, this facilitating a holistic understanding of the classroom dynamics. Beyond mere classification, our software includes standard statistical analysis of the learning styles, and incorporates advanced statistical methodologies, such as principal component analysis. Through these analytical techniques, the software allows the identification of the predominant learning styles. Furthermore, it elucidates how these styles interplay within student cohorts. To illustrate the potential of the application of CHAEA3S, we present results for the case of study of first-year university engineering students.

A Chatbot as a Virtual Assistant for the Students of the Introductory Course in Physics: A Case Study in an Online University

1st author

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Abstract

The first chatbot within the campus of an online university has been implemented and analyzed as a pilot in the Physics I subject with 66 students, with the aim of a first preliminary analysis for the deployment of the solution to other centers and degrees. The chatbot is based on commercial LLM API with prompt and temperature engineering adjustments, to reduce any prospect hallucinations. The profile of the number of

accesses to the virtual assistant showed a high concentration of accesses in a small group of students. A 5-point Likert scale questionnaire has been designed, validated, and answered by the students. The results obtained were: - Skill Development (Mdn=4.00, SD=0.58). Analyses the virtual assistant as a catalyst for the promotion of critical thinking and the improvement of research skills. - Virtual Assistant Interaction (Mdn=4.13, SD=0.64). Addresses two critical dimensions of human-computer interaction: usability and content relevance. - Technical and Accessibility Aspects (Mdn=4.25, SD=0.52). Covers ease of access, interaction experience, and efficiency in solving technical problems. - Efficiency of the Virtual Assistant (Mdn=4.25, SD=0.51). This evaluates the perceived usefulness of the assistant in the educational context, specifically in terms of its ability to facilitate understanding of subject concepts. - Impact on Learning (Mdn=4.25, SD=0.56). Evaluates the influence of this tool on student autonomy and retention of course information, as well as on the clarity and understanding of complex concepts. - Student Satisfaction (Mdn=4.63, SD=0.67). Assesses the student's overall perception of the integration and usefulness of the virtual assistant within the context of their course. The students' qualitative opinions were collected (via forum and an open question of the questionnaire), finding that user cases varied: from support for theoretical doubts to support for problem-solving.

Particular aspects of the teaching of Atomic, Nuclear and Particle Physics

1st author

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Abstract

The teaching of Atomic, Nuclear and Particle Physics (ANAPAP) has several specific aspects that makes it very different from other Physics subjects. In first place, it is impossible at present to visualize the phenomena involved and it will still be so in the foreseeable future. The observation must be made through observables measured at distances at which the interaction has no effect. The development of these subjects has been made through experiments, and there is no set of principles, postulates and laws that allow us to build from scratch a theoretical framework explaining the existing data. This makes the structure of these matters very different from the teaching of classical physics subjects. New concepts, as resonances, virtual particles and others which are not explained in elementary Quantum Mechanics courses, play a fundamental role in ANAPAP. In the second place, concepts of all classical subjects appear along the teaching of ANAPAP and are necessary to understand the physics involved. In the third place, instrumentation is fundamental in the production of data, and to grasp the importance of instrumentation performance is fundamental to understand discoveries. Finally, these ANAPAP knowledge and knowhow have a key role in modern technology, Medicine, and other subjects, from atomic clocks to radiotherapy, of which a physicist is assumed to know at least the basics. In this communication we discuss the relevant aspects that make ANAPAP subjects more difficult to teach to students compared to Classical Physics subjects, and why investigating novel pedagogical tools and methods is highly desirable.

Adaptando juegos de exploración a actividades de gamificación

1st author

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Abstract

En la actualidad estamos viviendo una época dorada de los juegos de tablero. Es pues lógico que cada vez se usen más los juegos de tablero en actividades de educación (serious games. Los juegos más usados suelen ser adaptaciones de juegos clásicos (parchís, bingo, Trivial Pursuit, etc) y juegos manipulativos como las escape rooms. Un nuevo tipo de juegos ha hecho aparición recientemente en el mundo de los juegos de tablero. Son los llamados juegos cooperativos de exploración, en los que los jugadores cooperan para cumplir ciertas misiones dentro de una narrativa embebida en el juego mientras exploran una región. Los jugadores adquieren los conocimientos y habilidades necesarias para ganar explorando la región en la que tiene lugar la narrativa. Así pues, la implementación de estas mecánicas de exploración en serious games permitiría a los jugadores adquirir conocimientos y aplicarlos en la misma partida: todo el proceso de aprendizaje se encuentra embebido en el juego. En esta presentación mostraremos resultados de dos Proyectos de Innovación Educativa [1,2], relacionados con la tecnología nuclear, la medicina nuclear, y la minería espacial en los que se desarrolló un librojuego [3] del tipo “Elige tu propia aventura” y un juego basado en las mecánicas de Cantaloop [4], que adapta las aventuras gráficas clásicas a un juego de tablero. Se explicará la metodología seguida para poder producir estos juegos, así como sus posibilidades para implementarlos en redes sociales, siguiendo ejemplos ya existentes [5].

[1] E. Oliva, et al, “Elige tu propia aventura... en Ingeniería Nuclear”

<https://innovacioneducativa.upm.es/proyectos-ie/informacion?anyo=2019-2020&id=3189>

[2] E. Oliva, et al, “The Secret of UPM Island”

<https://innovacioneducativa.upm.es/proyectos-ie/informacion?anyo=2023-2024&id=1125>

[3] E. Oliva. “Soles Rojos: Atrapado en la Antártida. Un librojuego sobre Tecnología Nuclear”.

http://ingenio.upm.es/permalink/f/1vo0cl5/34UPM_ALMA11181783750004212

[4] Friedeman Findeisen, “Cantaloop – Book 0, Book 1, Book 2, Book 3”, Lookout Games.

https://lookout-spiele.de/en/games/cantaloop_book1.html

[5] Samsung España, “¿Quién es el asesino?”

<https://twitter.com/SamsungEspana/status/1496125857068470273>

POSTER: Dificultades de aprendizaje de estudiantes de secundaria en el comprensión de eclipses

Presenter

Maddi Ortueta UPV/EHU

Co-presenters

Leire Arreal UPV/EHU

Kristina Zuza UPV/EHU

Abstract

El 12 de agosto de 2026 y el 2 de agosto de 2027 serán visibles dos eclipses totales de Sol desde diferentes puntos de España. Es de esperar que en la sociedad en general y en la enseñanza en particular se darán oportunidades para hablar, discutir y enseñar sobre eclipses. Teniendo en cuenta este escenario, se ha iniciado un proyecto que tiene como objetivo final diseñar una Secuencias de Enseñanza Aprendizaje (SEA) siguiendo la metodología Design Based Research (DBR). Para desarrollar esta metodología es necesario conocer las dificultades de los estudiantes en relación a los objetivos de aprendizaje.

Este trabajo es el primer paso para el diseño de la SEA mediante la metodología DBR, se presenta la investigación que se ha desarrollado para detectar las dificultades que tienen los estudiantes de secundaria para comprender el fenómeno de los eclipses. Se ha investigado sobre la comprensión de las fases de la luna, la relación entre estas fases y los eclipses, así como las diferencias y similitudes que hay entre los eclipses solares y lunares. Se ha diseñado un cuestionario abierto de diez preguntas que han respondido 450 estudiantes de secundaria de la provincia de Vizcaya.

Después de realizar un análisis fenomenográfico de las respuestas de los estudiantes siguiendo la metodología de Marton, se ha obtenido una categorización de las respuestas de los estudiantes y las dificultades que presentan. Estos resultados, muestran que los estudiantes tienen dificultades muy severas para comprender las fases de la luna y su relación con cómo se ve la luna desde la tierra (2,4% correctas) o para relacionar la fase de la luna con el tipo de eclipse (17% correctas). Los porcentajes de las respuestas correctas disminuyen para preguntas más específicas.



Physics of the Atmosphere and Ocean (GEFAO) / Física de la Atmósfera y del Océano (GEFAO)

Organiser

Juan A. Añel

Symposium abstract

The physics of the atmosphere and ocean explains a large part of the physical processes that occur on our planet, as well as on others. In this sense, it is the basis of disciplines such as meteorology, oceanography or climatology, with a very direct relationship with fluid dynamics. This symposium accommodates all communications related in one way or another to these topics. At the symposium, presentations are accepted to be presented orally or as a poster.

La física del atmósfera y del océano explica gran parte de los procesos físicos que ocurren en nuestro planeta, así como en otros. En este sentido es la base de disciplinas como la meteorología, oceanografía o climatología, con una relación muy directa con la dinámica de fluidos. En este simposio se da cabida a todas las comunicaciones relacionadas de una forma u otra con estas temáticas. En el simposio se aceptan presentaciones para ser expuestas de forma oral o como póster.

List of abstracts at the symposium

POSTER: Variación futura del régimen pluviométrico de Barcelona bajo escenarios de cambio climático por calentamiento global

Presenter

M. Carmen Casas Castillo Department of Physics, ESEIAAT, Universitat Politècnica de Catalunya-BarcelonaTech

Co-presenters

Ricard Kirchner Department of Physics, ESEIAAT, Universitat Politècnica de Catalunya-BarcelonaTech

Raúl Rodríguez-Solà Department of Physics, ETSEIB, Universitat Politècnica de Catalunya-BarcelonaTech

Abstract

Se han analizado series de lluvia futura proyectadas para los dos últimos tercios del siglo XXI en el Observatorio Fabra de Barcelona (noreste de la Península Ibérica), bajo diversos escenarios de cambio climático debido al calentamiento global, con el objetivo de evaluar posibles cambios en la complejidad y otras características del régimen pluviométrico del área estudiada. Este análisis se ha realizado en términos de parámetros fractales y multifractales específicos, obteniéndose pequeños cambios a esperar en el futuro. Por un lado, las series de lluvia futuras continuarán exhibiendo anti-persistencia, aunque en menor medida que actualmente. La anti-persistencia en las series significa que las fluctuaciones grandes suelen ser seguidas por otras más pequeñas y viceversa, lo que resulta en un retorno más rápido a la media en comparación con una serie con fluctuaciones aleatorias. Por otro lado, el 65% de las series proyectadas, tanto para la primera como para la segunda parte del siglo, muestran una ligera mayor complejidad que las históricas. En otras palabras, los modelos climáticos parecen estar proyectando un ligero aumento futuro en la complejidad de los mecanismos que conducen a la lluvia en el área estudiada debido al cambio climático.

POSTER: Comparison of different stratospheric parameters from reanalysis and satellite data

Presenter

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Co-presenters

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Rolando García National Center for Atmospheric Research

Martin G. Mlynczak NASA Langley Research Center

Abstract

In this study we compare various stratospheric parameters obtained from reanalysis and satellite data. The data from ERA5.1, MERRA2, JRA55, and JRA3Q reanalysis, as well as from the MLS and SABER satellite instruments are used to assess the agreement between reanalysis and satellite data in the stratospheric layer. In particular, the geopotential height of the tropopause and stratopause, as well as the stratospheric thickness, are computed and compared. The results show that the most significant discrepancies are observed in the tropics (30°S to 30°N) and the global mean, where negative correlations with satellite data are found. The correlations in the southern hemisphere extratropics are lower than those in the northern hemisphere extratropics. Moreover, the stratospheric thickness, a priori expected to be well-correlated with the stratospheric temperature, not always behaves this way.

POSTER: Impacto del cambio climático en la estructura, propiedades dinámicas y espesor de la estratosfera

Presenter

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Abstract

El cambio climático tiene un impacto significativo en la estructura y propiedades de la atmósfera terrestre por encima de la tropopausa. Los efectos más notables incluyen una disminución de la temperatura y la densidad. Sin embargo, es difícil establecer tendencias para esta región de la atmósfera, que incluye la estratosfera y superiores. Esto se debe principalmente a la necesidad de conjuntos de datos a largo plazo para garantizar que las tendencias sean sólidas y estadísticamente significativas. También es necesario considerar el impacto de la influencia solar al intentar cuantificar el papel de las emisiones antropogénicas en las tendencias de diversas variables.

En este estudio, exploramos todas estas cuestiones, incluidos los efectos de diferentes métricas en la cuantificación y tendencias como las diferencias en los niveles geopotenciales, la temperatura, la densidad y el ancho de las capas. Para lograr esto, utilizamos una combinación de reanálisis y datos satelitales. Los resultados tienen en cuenta los valores medios globales y las diferencias latitudinales. Observamos una contracción y enfriamiento de la estratosfera en todas las capas, pero con algunas variaciones.

POSTER: La basura espacial y la necesidad de una mejor vigilancia del cambio climático en la media y alta atmósfera

Presenter

Juan Antonio Añel Cabanelas EPhysLab, Universidade de Vigo

Co-presenter

The ISSI Team #544 -- International Space Science Institute

Abstract

Las emisiones antropogénicas de gases de efecto invernadero tienen efectos importantes en la atmósfera media y superior. El aumento de las concentraciones de gases de efecto invernadero provoca que la atmósfera media y superior se enfríe y también puede provocar cambios en la circulación. El enfriamiento de la atmósfera media y superior provoca varios efectos secundarios importantes asociados con la contracción térmica, como cambios en la estructura vertical de la atmósfera, incluida la contracción estratosférica, la estructura de densidad electrónica ionosférica y una disminución en la densidad de la termosfera en alturas fijas. La reducción a largo plazo de la densidad de la termosfera prolonga la vida natural de los objetos en órbita baja, lo que agrava el problema de la acumulación de basura espacial. La ionosfera afecta la propagación de señales de radio, como las utilizadas por las comunicaciones de larga distancia y los sistemas de posicionamiento global por satélite. A largo plazo, las características de las irregularidades ionosféricas que dan lugar al centelleo y a las frecuencias máximas utilizables para comunicaciones podrían sufrir cambios sutiles. Esto tiene implicaciones para el futuro en cuanto a basura espacial, la política espacial y la industria de seguros. Sin embargo, la disponibilidad limitada de conjuntos de datos completos y precisos que permitan un análisis de las tendencias a largo plazo impide una evaluación adecuada de la situación y las amenazas que plantean estos fenómenos. Lamentablemente, la disponibilidad de observaciones de la atmósfera media y superior adecuadas para el análisis de tendencias a largo plazo se está deteriorando en lugar de mejorar.

POSTER: Ozono superficial semicuantitativo de los siglos XIX y XX a lo largo de la Europa subtropical hasta las costas atlánticas de África tropical

Presenter

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Abstract

Los registros del ozono troposférico en la Tierra antes de finales del siglo XIX son escasos. El estudio del ozono troposférico enfrenta dos desafíos principales: la falta de registros preindustriales dificulta la comprensión de las tendencias climáticas a largo plazo, dado el papel crucial del ozono en los modelos climáticos y existen incertidumbres sobre sus valores en una atmósfera no contaminada en todo el planeta. El ozonoscopio fue el primer instrumento utilizado para medir el ozono. A pesar de su vulnerabilidad a la humedad y los niveles de oxidantes, ofrece estimaciones semicuantitativas del ozono en superficie cuando

no había otras mediciones disponibles. A pesar de su valor potencial, la digitalización, conservación y publicación de datos de ozonoscopios sigue estando en gran medida inexplorada. En este trabajo iniciamos un esfuerzo por rescatar los registros del ozonoscopio de ozono en superficie. Aquí incluimos datos de 24 observatorios que cubren Portugal y el sector atlántico africano, proporcionando un rango latitudinal desde los extratrópicos en el hemisferio norte hasta los trópicos en el hemisferio sur e introduciendo la serie de datos de ozonoscopio más larga conocida hasta la fecha, que abarca 50 años de observación diaria.

Medical physics (GEFM) / Física Médica (GEFM)

Organiser

Gabriela Llosa

Invited speakers

Jordi Llop (CIC BiomaGUNE) José Miguel Delgado (Presidente de la Sociedad Española de Radiocirugía) Jorge ROSER (Institute Of Medical Engineering, Universität Zu Lübeck) Ane ETXEBESTE (Université de Lyon- CREATIS)

Symposium abstract

The RSEF specialized group symposium on Medical Physics, which will take place at the XXXIX Biennial Meeting, aims to be a forum to relate researchers in this field and communicate advances in Medical Physics in its different lines of research: control quality of radiotherapy treatments with both photons and hadrons; development of detectors for imaging and dosimetry; image reconstruction and analysis and importance of AI in its reconstruction; radiomics and many other topics that are positioned every day in this specialty due to advances in other areas of Physics that impact the development of Medical Physics.

El simposio de grupo especializado en Física Médica de la RSEF, que va a desarrollarse en la XXXIX Reunión Bienal tiene como objetivo ser un foro para relacionar a los investigadores en este campo y comunicar los avances en Física Médica en sus distintas líneas de investigación: control de calidad de los tratamientos de radioterapia tanto con fotones como con hadrones; desarrollo de detectores para imagen y dosimetría; reconstrucción y análisis de imagen e importancia de la IA en su reconstrucción; radiómica y otros muchos temas que cada día se posicionan en esta especialidad por los avances en otras áreas de la Física que repercuten en el desarrollo de la Física Médica.

List of abstracts at the symposium

Promises and limitations in the present and future of radiotheranostics: from self-propelled nanosystems to controlled metabolism

1st author

Jordi Llop CIC biomaGUNE

Abstract

Theranostics is an innovative nuclear medicine technique that uses radioactive drugs to both diagnose and treat cancerous tumours. This approach involves using one radioactive drug for imaging and diagnosis, followed by a second radioactive drug for therapy. The recent clinical success of theranostic pairs has generated new opportunities and optimism, prompting major pharmaceutical companies and biotech firms to investigate targeted drugs that deliver both diagnostic and therapeutic radionuclides to tumours. Despite these advancements, significant challenges remain in translating promising preclinical candidates to clinical settings. Key issues include insufficient accumulation and retention of radiolabelled drugs in tumour tissues and their unwanted accumulation in non-target organs, which can lead to adverse side effects. This presentation will provide an overview of the theranostics concept, showcasing recent successful applications. It will also address the major limitations and necessary improvements in the field. Additionally, our work on the use of self-propelled nanobots for personalized medicine in bladder cancer will be discussed, highlighting potential future strategies to mitigate off-target toxic effects.

Hyperspectral imaging and deep learning for medical diagnosis

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Abstract

Hyperspectral imaging has emerged as a promising technology for diagnostic purposes in various medical applications where both spectroscopic and morphological information of the samples under analysis is crucial. Additionally, the integration of machine learning algorithms with imaging modalities is anticipated to revolutionize medical diagnosis in the upcoming years. In this conference, we will present our most recent achievements in these fields with the aim of improving the diagnosis of several diseases [1-3]. Firstly, we will describe multiplexed staring hyperspectral imagers developed to improve non-invasive diagnosis of skin cancer and eye fundus diseases. These systems consist of silicon and InGaAs sensors, as well as light-emitting diodes, which allow acquiring visible and near-infrared images of skin lesions (including nevi, melanomas, and basal cell carcinomas) and the eye fundus at various wavelengths, highlighting spectral signatures of components of the biological tissue. Secondly, we will present our latest study using hyperspectral technology alongside confocal laser scanning microscopy, enabling spectral and 3D characterization of cells simultaneously, to refine the diagnosis of blood diseases. Specifically, we focus on hemoglobinopathies (such as thalassemia and sickle-cell disease) and cell membrane disorders like hereditary spherocytosis. In this study, we designed immunolabeling protocols targeting different membrane proteins and analyzed hyperspectral fluorescence images to distinguish between healthy and diseased red blood cells. Moreover, we will explore new insights utilizing Computer-Aided Diagnosis based on customized Deep Learning algorithms featuring 2D (conditional variational autoencoders) and 3D convolutions to process the spectral image cube as a whole (VGG-16). These algorithms are trained to classify healthy and diseased biological samples using hyperspectral datasets, marking a significant advancement in medical diagnostics. Acknowledgements: Funded by MCIN/AEI/10.13039/501100011033 (PID2020-112527RB-I00) and the European Union (HORIZON-MSCA-2022-DN, GA n°101119924-BE-LIGHT).

[1] Biomedical Optics Express 13(6), 3504 (2022)

[2] Microscopy and Microanalysis 29(2), 777 (2023)

[3] SPIE Proc. 12627, 1262706 (2023)

Towards tissue-targeted disease detection on a low-field portable scanner using quantitative brain maps

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Abstract

Quantitative Magnetic Resonance Imaging sequences is frequently the Gold-Standard for disease detection, thanks to it's sensitivity to subtle changes in tissues properties, induced by lesions. However, conventional MRI scanners are very resource and time demanding, becoming inaccessible to a vast part of the population. This is why we present a initial fingerprinting-based approach to quantitative brain mapping for singular tissue detection, in hopes of implementing it on an upcoming ultra-portable low-field scanner. Parallel to scanner's construction, we simulated a fingerprinting process to generate quantitative brain maps, using publicly available brain phantoms to which we generated MS lesions in their White Matter. We optimized different lengths of TR/FA schedules (10, 30, 60 and 120 pairs of TR/FA's) using the 3 tissues of the brain we considered (Grey Matter, White Matter and MS) with Julia programming language BlackBoxOptim. We then tested the accuracy of each one in a simulated 2D ZTE sequence, with varying degrees of undersampling. Dictionary generation and matching was performed using Matlab 2023b. Validation parameter to determine the best compromise between accuracy and scanning time was a comparison of the estimated MS surface of each slice and the phantom. We observed that accuracy in MS quantity is mostly dependent on the undersampling, showing a steep degradation when it becomes higher than 10 times, remaining stable up to that point. However, a too-small schedule can also hinder the MS detection ability. We established the acquisition of 40 spokes and schedule length of 30 as the best compromise between accuracy and scanning time. This schedule highlights that optimal detection of particular tissue can be much faster than generic quantitative mappings of all tissues, paving the way for optimized tissue-targeted fingerprinting sequences. Once the scanner construction is completed, we will test its performance experimentally.

Low-field portable MRI scanner with an elliptic-bore Halbach magnet

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Abstract

One first goal of this work is to improve the main magnetic field and portability of low-field MRI scanners to reach home and hospice care, small clinics, rural areas, NGO camps, etc., making MRI available to a large

fraction of the world's population with no or insufficient access. A second goal is to improve the accessibility and adjustment of patients with an elliptic Halbach magnet configuration [1]. Elliptic Halbach geometries allow us to place human extremities and can make our systems suitable for neuroimaging. The main magnet is made of 19 polyethylene rings which have been machined to contain cubic Nd₂Fe₁₄B magnets. Every ring is covered with a machined 2.5 mm thick laser-cut aluminum plate. Similarly, the shimming unit is composed of 23 polyethylene rings, with CNC machined sockets and threaded rods for fastening. The gradient module consists of four concentric elliptical lobes that span the full-length of the magnet. Every gradient coil lobe is a water-jetted copper plate curved and later fixed to his support. All these components are housed in an aluminum structure designed to withstand the magnet and all associated electronic components weight. This structure measures 68 x 95 x 140 cm³ (width x height x length). Everything required to run the scanner except power generation is contained inside so it can be used as a standalone device. The magnet generates a magnetic field of 87 mT, homogeneous down to 5,700 ppm in a 20 cm diameter FoV. We have achieved a truly portable Halbach magnet scanner with an elliptical bore amenable to heads and large feet with full-length gradient support, which fits through doors and weighs around 400 kg.

1. Galve, F., Pallás, E et al (2024, March 12). Elliptical halbach magnet and gradient modules for low-field portable MRI. arXiv.org. <https://arxiv.org/abs/2403.07761>

First validation of a trimodal imaging system: PET-FUS-MR

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Abstract

The integration of Positron Emission Tomography (PET) scanners with Magnetic Resonance (MR) and/or Focused Ultrasound (FUS) devices has emerged as a leading approach in different medical areas such as oncology and neurology.

Recently, it has been proposed combining the three modalities in a single system to provide simultaneous PET/MR images while applying the FUS. One of the most exciting applications for such a trimodal system

is using FUS to open the Brain Blood Barrier (BBB) to allow drug deposition inside the brain and enhance treatment while simultaneously acquiring PET/MR data to provide functional and anatomical images, respectively.

Note that, to date, there is none trimodal system available. To cover this gap, we have designed, assembled and validated a small-animal preclinical PET insert compatible with both FUS and MR systems. This report details the initial performance evaluation of our PET system, following the NEMA NU 4 2008 standards. We have achieved spatial resolution values of 0.9 mm FWHM, sensitivity of 3.1% within a 30% of energy window, and the noise equivalent count rate (NECR) peak was 92 kcps at 600 uCi. Moreover, we have reconstructed the Image Quality (IQ) phantom and obtained: (i) Recovery coefficients (RC) of 0.17, 0.38, 0.90, 1.08 and 1.04 for rods ranging from 1 mm to 5 mm, respectively; (ii) image uniformity of 4.3% and; (iii) spill-over values of 22.9% in water and 15.1% in air.

For the first time, we present a trimodal PET-MRI-FUS study. Using FUS, we heated a gelatin-filled phantom containing FDG in a specific area. Throughout the heating process, different MR sequences were running and PET data was being acquired. As the gelatin melted, the FDG was distributed within the entire phantom cavity. This dispersion was observed in the reconstructed images, thus validating our trimodal system.

Advanced preclinical PET scanner based on semi-monolithic detectors with TOF and DOI capabilities

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Abstract

Semi-monolithic crystals have the potential to combine the timing capabilities of pixelated detectors and the 3D position accuracy of monolithic crystals.

We present a PET scanner for small animals consisting of 2 rings of 14 detectors based on arrays of semi-monolithic crystals. The inner diameter is 106 mm and the axial length is 52 mm. Each detector contains 22 slabs (0.97x25.6x12 mm³), optically isolated with ESR, a retroreflector layer on the top face and black paint on the lateral ones. The detectors are coupled to an 8x8 SiPMs array with 3x3 mm² active area each, and all channels are individually readout using the TOFPET2 ASIC from PETsys.

Different calibration techniques were applied to achieve a mean energy resolution of 20.9 ± 1.8 % at system level. The timing resolution of one detector was studied, applying time skew, time walk corrections and a timestamp averaging method. A Detector Time Resolution (DTR) as good as of 178 ps at the center of the detector was obtained.

A supervised Neural Network (NN) based on a multilayer perceptron (MLP) was used to estimate the impact position along the monolithic coordinate. The DOI coordinate was determined using the Energy/*I*_{max} estimator.

A spatial resolution of 0.96 ± 0.07 mm was achieved at $\frac{1}{4}$ of the axial FOV, worsening to 1.4 ± 0.3 mm when no DOI information is used. A 3.1% sensitivity was determined at the center of the scanner, with a 30% energy window. A NECR value of 10 kcps at a 280 μ Ci activity was achieved.

Additionally, recovery coefficients (RC) and Spill-Over-Ratio (SOR) values were calculated for the NEMA image quality phantom, yielding RCs of 0.08, 0.47, 0.67, 0.79, and 0.88 for 1, 2, 3, 4, and 5 mm rods, respectively, together with SOR values of 0.18 for air and 0.27 for water.

Obtención simultánea de imágenes PET de dos radiotrazadores en estudios dinámicos

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Abstract

En investigaciones previas [1], se logró la obtención simultánea de imágenes cuantitativas de dos radiotrazadores PET mediante la detección de la aniquilación positrón-electrón y las emisiones gamma inmediatas para imágenes PET. El uso de radiotrazadores con mecanismos de captación específicos y distintos, posibilita el análisis simultáneo de múltiples procesos biológicos. Por ejemplo, en oncología, esta técnica podría mejorar la caracterización de tumores, la evaluación de la respuesta al tratamiento y la identificación de biomarcadores predictivos. Para ello, el método propuesto implica el uso de dos tipos de emisores beta: uno puro (^{18}F , ^{68}Ga , etc) que emite un único positrón durante su decaimiento beta, y otro que, además del positrón, emite un gamma adicional, permitiendo su identificación durante el procesamiento de datos (^{124}I , ^{86}Y , etc). Las imágenes obtenidas tras la separación resultaron satisfactorias para adquisiciones estáticas, de modo que el siguiente objetivo es ampliar su aplicación a adquisiciones PET dinámicas, lo que permitirá investigar la farmacocinética de los radiotrazadores en diferentes regiones de interés.

En el presente estudio, se describe el flujo de trabajo y se presentan los resultados de adquisiciones reales realizadas en ratones a los que se les inyectaron ^{18}F -NaF y ^{124}I . Además de un análisis cualitativo de las imágenes de ambos isótopos en cada frame, se mostrarán las curvas de actividad para distintas regiones de interés correspondientes a ambas distribuciones de actividad como la vena cava, la vejiga, el estómago y la tiroides.

[1]: Pratt, E. C., Lopez-Montes, A., Volpe, A., Crowley, M. J., Carter, L. M., Mittal, V., ... & Herraiz, J. L. (2023). Simultaneous quantitative imaging of two PET radiotracers via the detection of positron-electron annihilation and prompt gamma emissions. *Nature Biomedical Engineering*, 7(8), 1028-1039.

Avances en la integración tecnológica en Radiocirugía

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Abstract

Una de las formas reconocidas de tratamiento local del cáncer es la terapia con radiaciones que ha experimentado en las últimas décadas un desarrollo espectacular y se encuentra en este momento en una encrucijada debido a la cantidad de tecnología que se está desarrollando a medida que se encuentran nuevas formas de abordar las lesiones. Un problema para la decisión de adquisición tecnológica de los próximos años es la compatibilidad de disponer de todos los desarrollos que se han venido produciendo en la última década con un moderado coste de inversión. Estamos en un momento donde la terapia Flash, la terapia adaptativa, y la integración de las tres formas básicas de producción de imágenes tomográficas (CT, PET, MR) en las unidades de irradiación constituidas por aceleradores lineales. Por otro lado, el desarrollo de los aceleradores de protones y su aproximación, tanto en tamaño físico, como económico sugieren un desarrollo de diferentes terapias muy atractiva, especialmente con la reciente adquisición en el estado español de un conjunto importante de máquinas. En contraposición están apareciendo nuevos aceleradores VHEE con energías de electrones entre 50-200MeV y con capacidad para ser focalizados y escaneados fácilmente y que proporcionan tasas de emisión ultra altas(40-100Gy/s). Estas máquinas permitirán terapias Flash con la aparición de nuevas estrategias con otros tipos de tratamiento, Inmunoterapia, teragnostic, etc. Ninguno de estos sistemas avanzará por si solo, si los otros elementos complementarios en un sistema radioterápico no se desarrollan concomitantemente con ellos. Los nuevos procesadores y la incorporación de la IA a los procesos de planificación serán imprescindible para sacar rendimiento a estas nuevas formas de emisión de radiación. Naturalmente debemos de desarrollar una forma más rápida de dosimetría física y en tiempos real. El objetivo de esta presentación es analizar las posibilidades de integración de estas tecnologías en los servicios asistenciales y especialmente en el ámbito de la Radiocirugía tanto intracraneal (SRS) como corporal (SBRT).

Premio tesis GEFM: Improving the image quality with Compton cameras for medical application

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Abstract

Improvement of the image quality that can be attained with Compton cameras is one of the main requirements for their implementation in medical applications such as online range verification in hadron therapy, where the use of imaging devices capable of coping with high, multi-energy gamma-rays can be advantageous. In this work, several software-based approaches to improve the quality of the images obtained with Compton cameras are introduced. The performance of these approaches is demonstrated by using experimental data acquired with MACACO, the Compton camera under development at the IRIS group of IFIC-Valencia. The results show that the developed techniques improve MACACO's capability of detecting shifts of the proton depth-dose distribution at clinical energies, as well as demonstrating its potential for radiopharmaceutical imaging of phantoms and patients in the context of nuclear medicine.

Assessment of dose distributions by alpha-, beta- and Auger-emitting radioisotopes by means of simple yet reasonably accurate Monte Carlo simulations

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Abstract

Targeted radionuclide therapy is a powerful technique for treating cancer [1], in which antibodies are linked to alpha-, beta- or Auger-emitting radioisotopes, accumulating inside malignant cells. The emitted radiations, of different penetration ranges, are suitable for treating extended tumors or small cell-scale metastases. Apart from the macroscopic doses, it is important to accurately assess their energy deposition profiles at the nanometre scale, as the biological outcomes of radiation result from complex lesions induced in DNA molecules [2].

In our group, we develop detailed models (based on the dielectric formalism [3]) for calculating accurate integral and differential inelastic cross sections for energetic ions and electrons in biomaterials [4-5]. Such results can be parametrised by analytical approximations [6], which are easy to implement in Monte Carlo codes and maintain simplicity and speed of calculation. We will present results of Monte Carlo codes we have developed to follow in detail the motion of electrons and alpha particles through liquid water, based on analytical elastic and inelastic cross sections. Their performance will be assessed, for representative electron- (e.g. ^{131}I , ^{125}I) and alpha-emitting (e.g. ^{211}At , ^{223}Ra) isotopes, by comparison to reference simulations [7, 8].

[1] V. Radchenko, C. Hoehr, *Nuclear Physics News* 30 (2020) 28

[2] A. V. Solov'yov (ed.), *Nanoscale Insights into Ion-Beam Cancer Therapy*, Springer (2017)

[3] I. Abril, R. Garcia-Molina, C. D. Denton, F. J. Pérez-Pérez, N. R. Arista, *Physical Review A* 58 (1998) 357

[4] P. de Vera, R. Garcia-Molina, I. Abril, *Physical Review Letters* 114 (2015) 018101

[5] P. de Vera, I. Abril, R. Garcia-Molina, *Physical Chemistry Chemical Physics* 23 (2021) 5079

[6] P. de Vera, I. Abril, R. Garcia-Molina, *Frontiers in Materials* 10 (2023) 1249517

[7] N. Falzone et al., *Physics in Medicine and Biology* 62 (2017) 2239

[8] R. Peter et al., *Scientific Reports* 12 (2022) 17934

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Radiobiological effects of laser-generated protons and X-rays in cell cultures

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Abstract

Particle sources based on ultra-intense laser-plasma interactions offer unique conditions to study the response of biological systems to ionizing radiation at instantaneous dose rates orders of magnitude higher than those from radiofrequency accelerators. We have run two experimental campaigns which, on the national level, have been the first combining laser-driven sources with radiobiology research.

A stabilized X-ray source has been realised at the Laser Laboratory for Acceleration and Applications (L2A2, Santiago de Compostela). A 35 fs pulsed laser with 1 mJ pulse energy at 1 kHz shot rate is focalized on a rotating copper plate. It generates bremsstrahlung up to some tens of keV. Total doses ranging from 3 to 8 Gy has been delivered to 36 monolayer cell cultures of human lung adenocarcinoma (A549) prepared at Instituto de Investigación Sanitaria (IDIS). At 10 cm target distance the average dose rate is about 100 mGy/s. The applied dose is measured with radiochromic films. An ionization chamber has been implemented for real-time dose control.

Our first experiment on biological effects of laser-accelerated protons has been run at Centro de Láseres Pulsados (CLPU, Salamanca). A three-axis controlled wheel, developed by IGFAE, has been applied for the precise positioning of 808 individual targets per vacuum cycle in the focal spot of the VEGA-3 laser (1 PW, 27 J at 1 Hz pulse rate). A magnetic energy selector from i3M has been implemented to obtain a quasi-monoenergetic proton beam which was guided through a thin vacuum window. A total of 27 cell samples, prepared by Instituto de Biología Funcional y Genómica (IBFG), have been exposed to tens of nanosecond proton pulses accumulating total dose values between 3 and 8 Gy.

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Reconstrucción de Dosis 3D en Protonterapia Usando Redes Neuronales Profundas y Detección de Emisores de Positrones

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Abstract

La protonterapia se ha consolidado como la opción de tratamiento preferente para tumores pediátricos, cerebrales y otros de difícil acceso. La instalación de diez nuevos centros, sumados a los tres existentes, situará a España como un referente europeo en este campo. Sin embargo, para maximizar los beneficios de esta terapia, es crucial identificar desviaciones en la deposición de dosis que puedan dañar tejido sano. Ante la incapacidad de medir la dosis depositada directamente, dado el recorrido finito de los protones,

existe la posibilidad de medir la activación, o distribución de emisores de positrones activados por el haz de protones, con un dispositivo PET.

Nuestro trabajo, por primera vez, introduce una herramienta basada en GPU y redes neuronales profundas en 3D para predecir la deposición de dosis a partir de la activación. Implementamos esta herramienta en un plan de tratamiento de cáncer de próstata, introduciendo desviaciones posicionales y de densidad clínicamente realistas. Evaluamos los resultados obtenidos con tres arquitecturas de redes neuronales convolucionales: *SegResNet*, *UNet*, y *SwinUNETR*.

Todos los modelos demostraron una alta precisión, prediciendo la dosis depositada con un *Gamma Passing Rate* superior al 99.99% y reduciendo el error cuadrático medio a una milésima parte del obtenido comparando la dosis depositada al introducir desviaciones respecto al plan de referencia. Además, los modelos son capaces de predecir las desviaciones posicionales con una precisión superior a 0.1mm y 0.1°.

El proceso completo, desde la adquisición de datos a partir del plan de tratamiento hasta el entrenamiento de las redes, se puede completar en menos de dos horas usando una GPU. La herramienta presentada podría ser útil para detectar desviaciones críticas en el tratamiento que sean corregidas en el momento o en las siguientes sesiones.

Reducción de ruido en imagen 3D con cámaras Compton usando discretizaciones no uniformes del campo de visión

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Abstract

La imagen de rayos gamma de emisión rápida (PG) con cámaras Compton ha suscitado interés como una posible herramienta para la verificación del rango en terapia hadrónica. No obstante, la baja proporción de señal a ruido suele degradar las imágenes obtenidas con esta técnica, dificultando así la detección de posibles desplazamientos de las distribuciones de PG. En este trabajo buscamos mejorar la calidad de la imagen en la región de interés (ROI), es decir aquella donde se espera localizar la distribución de PG, con el objetivo de mejorar la identificación de dichos desplazamientos.

Con este fin, hemos simulado en GATE 9 un paralelepípedo rectangular emisor de rayos gamma con energía 4.44 MeV, y una cámara Compton con tres cristales centelleadores de LaBr3. Las imágenes fueron obtenidas mediante el algoritmo LM-MLEM, por una parte usando vóxeles uniformes, y por otra usando una discretización no uniforme con vóxeles progresivamente más grandes hacia los límites del campo de visión (FOV). En ambas discretizaciones se usó el mismo número de vóxeles.

Los resultados muestran una mejora del contraste en las imágenes obtenidas con la discretización no uniforme del FOV, junto a una mejora del 26.5 % en la identificación del extremo distal de las distribuciones simuladas. También se observa una mejora del NRMSD, indicando imágenes cuantitativamente más próximas a las distribuciones simuladas y con menor ruido.

Así pues, el presente trabajo muestra que el uso de una discretización no uniforme del FOV puede mejorar la calidad de las imágenes 3D obtenidas con una cámara Compton. La siguiente fase de esta investigación incluye el diseño de discretizaciones del FOV mejor adaptadas así como la evaluación de los límites de la técnica.

Este trabajo ha sido financiado en parte por la Fundación Alemana de Investigación (DFG), proyecto COMMA, número 383681334.

Monte Carlo simulation of the water equivalent ratio in condensed-phase materials of interest in protontherapy

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Abstract

Hadrontherapy has several advantages over conventional radiotherapy, such as the great targeting precision of the ion beams, due to their reduced angular scattering and their characteristic depth-dose curve, depositing a large fraction of their energy by the end of their trajectories. Therefore, ions (most commonly protons) are optimal particles to treat deep-seated tumors minimizing damage on the surrounding healthy tissues, and understanding the basic physical interactions is essential to maximize the induced sub-cellular damaging processes [1]. This work shows depth-dose distributions of swift proton beams interacting with biologically relevant materials (liquid water[2,3], cortical bone[4]), obtained with the SEICS (Simulation of Energetic Ions and Clusters through Solids)[3] code, which considers the energy loss due to inelastic and elastic collisions, as well as the fragmentation nuclear reactions and the projectile electron capture and loss processes. It uses accurate stopping power and energy-loss straggling values obtained using the MELF-GOS (Mermin Energy-Loss Function – Generalized Oscillator Strengths) method, which gives a detailed description of the electronic excitation spectrum of the condensed-phase targets[2, 3]. Simulations for relevant energies in protontherapy (tens and hundreds of MeV) compare very well with reference simulations and experimental data for Bragg curves, both in liquid water and cortical bone. The derived water equivalent ratio values for cortical bone are in reasonable agreement with recent determinations[5].

[1] D. Schardt, T. Elsässer, D. Schulz-Ertner, Rev. Mod. Phys. 82, 383 (2010).

[2] P. de Vera, I. Abril, R. Garcia-Molina, Radiat. Res. 190, 282 (2018).

[3] R. Garcia-Molina, I. Abril, S. Heredia-Avalos, I. Kyriakou, D. Emfietzoglou, Phys. Med. Biol. 56, 6475 (2011).

[4] S. Limandri, P. de Vera, R.C. Fadanelli, L.C.C.M. Nagamine, A. Mello, R. Garcia-Molina, M. Behar, I. Abril, Phys. Rev. E 89, 022703 (2014).

[5] A. L. Burin, I.S.L. Branco, H. Yoriyaz, Radiat. Phys. Chem. 203, 110606 (2023).

Monte Carlo study of the relation between lineal energy and restricted linear energy transfer for protons and carbon ions

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Abstract

The physical background of the relative biological effectiveness (RBE) of heavy charged particles has been modeled either by means of linear energy transfer (LET) and microdosimetric stochastic quantities, especially lineal energy. For a given particle energy and sites of sufficient size, the frequency-mean lineal energy (yF) is equal to the restricted track-averaged LET (LET_t), although the restriction value fulfilling this equality has not been parametrized to our knowledge. Same happens with the site size at which that equality does not hold. For these reasons, in this work we study the relation between these quantities for protons and carbon ions in water at therapeutical energies.

The Monte Carlo simulations were carried out with the Geant4 toolkit (v11.1.2), using the physics list G4EmDNAPhysics_option2 of the Geant4-DNA extension. Protons and carbon ions at energies up to 300 MeV/u were simulated with two different codes developed in our group: one for the calculation of restricted LET_t, and another [1] for the calculation of yF with spherical sites from 1 to 50000 nm in diameter.

The restricted LET_t was obtained as function of the radial distance to the core of the charged-particle track, observing an expected increasing trend with respect to the radial restriction until the LET_t became unrestricted; this value was checked with electronic stopping power values published at the ICRU90 report. When comparing restricted LET_t values with yF values obtained at same energy with different site diameters, we observed a good agreement for the largest diameters and radial restrictions of the LET. The diameter value at which the yF values did not match the trend observed for restricted LET_t was estimated for each energy to set the lower limit at which the yF values cannot be associated with a radially restricted LET.

[1] A. Baratto-Roldán et al., Front. Phys. 9: 726787 (2021).

Status of MACACO and FALCON Compton cameras for medical applications.

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Abstract

The IRIS group of IFIC (Valencia) has developed a Compton camera for monitoring and assessment of cancer treatments. As research advances, the system evolves to meet the specific requirements of each of the areas in which it has been tested. In protontherapy treatment monitoring, two systems, MACACOIII and

MACACOp, both composed of LaBr₃ crystals coupled to SiPM arrays, were tested at Krakow protontherapy centre. With both systems it was possible to distinguish 2 mm variations in the proton range by reconstructing the distribution of prompt gammas emitted upon irradiation of a RW3 phantom at different energies. Next, tests were conducted at Quirón protontherapy centre (Madrid), where the faster readout time of MACACOp has allowed to visualize the distribution of emitted photons in this challenging scenario. The system efficiency has been enhanced by enlarging the second detector plane in the prototype known as FALCON, which has been employed in further tests at Quirón.

In the assessment of radionuclide therapy, MACACOIII showed promising results in visualizing Derenzo-like phantoms filled with FDG and ¹³¹I-Nal, and also metastatic lesions in thyroid cancer patients, in collaboration with La Fe hospital (Valencia). The system has also been able to obtain an image with Ac-225 at Léon Bérard hospital (Lyon), which was not possible with the gamma cameras. The second plane of this system has also been enlarged to enhance the efficiency, and the prototype MACACO III+ has been able to image a thyroid-shaped phantom filled with ¹³¹I-mIBG, including a uniform background with hot spots in La Fe hospital

Basque Research and Technology Alliance (BRTA) at CIC biomaGUNE

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Abstract

The field of nuclear magnetic resonance (NMR) has witnessed several advancements in recent years, including the integration of artificial intelligence and machine learning, which has led to more efficient data analysis and interpretation. Additionally, there is a growing demand for portable and benchtop NMR systems, which offer convenience and ease of use in various applications. As a result, NMR spectroscopy and imaging have opened up new possibilities and benefits for physicists, chemists, and engineers, particularly in material science, medical diagnostics, and fundamental research. Low-field NMR offers several distinct advantages and applications that have never been explored before, making it an attractive option for experimental flexibility and accessibility in a variety of settings, from remote fieldwork to compact laboratory spaces.

This presentation will focus on the benefits of employing low-field NMR for metabolomics and imaging, highlighting how it can enhance sensitivity and detection capabilities and create novel applications. Several novel innovations in magnet design, pulse sequence development, and other technologies have significantly improved the sensitivity and resolution of low-field NMR systems. The aim of this presentation is to inspire innovative applications across diverse research domains by leveraging the specific advantages of low-field operation. By expanding the boundaries of their experimental toolkit, physicists can foster new discoveries and technological advancements. These advantages have the potential to transform the way NMR is conducted because low-field magnets are significantly less expensive, have lower maintenance costs, occupy less space, and are more accessible than their high-field counterparts.

Real-time time-dependent density functional theory of electronic stopping power for protons and antiprotons in LiF using plane waves

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Abstract

For many years, lithium fluoride (LiF) has been considered a crystal of interest from a fundamental point of view to understand the interaction processes of ionizing radiation with matter as well as from a practical point of view due to its use as a dosimeter to measure absorbed dose in occupational personal dosimetry, environmental monitoring, and medical and space dosimetry. The capability of a charged particle to lose energy to electrons per unit length traveled into matter is quantified by the electronic stopping power (SP). Experimental studies about the interaction of protons with LiF have reported that the SP vanishes below a velocity threshold of 0.1 a.u. Real-time time-dependent density functional theory (rt-TDDFT) simulations have confirmed the results for protons. However, for the antiprotons of low velocities where only rt-TDDFT data exist, the results are still controversial. For antiprotons, a similar velocity threshold and the Barkas effect (SP of the antiproton is lower than that of the proton) have been obtained from simulations using atomic orbitals. Results from rt-TDDFT using Gaussian basis sets in channeling trajectories suggested a negative Barkas effect (SP for antiprotons greater than that for protons) at velocities below 0.25 a.u. and, remarkably, no velocity threshold for antiprotons. This work presents SP results for protons and antiprotons in LiF via rt-TDDFT simulations using plane-wave methods. Incommensurate trajectories are used for both particles as a way to approach the effective trajectory averaging in experiments. Good agreement with available experimental data is obtained for both protons and antiprotons. A similar threshold effect is observed for both, with no trace of the reported anti-Barkas effect in the low-velocity limit. The results will be presented and discussed. We acknowledge computational support from Atlas DIPC, Spain, and Miztli UNAM Mexico through grant ref. LANCAD-UNAM-DGTIC-334. This project is partially supported by the European Commission Horizon MSCA-SE Project MAMBA (Grant No. 101131245). GMJL is on sabbatical leave at CIC-Nanogune in Spain funded by DGAPA UNAM

A new time-structure computational tool for microdosimetric studies of radiopharmaceutical therapy using TOPAS toolkit

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Abstract

Radiopharmaceutical therapy (RPT) is a novel modality of oncology treatments that uses radiolabeled agents affine to biomolecules overexpressed in tumor cell environments. Alpha emitter RPT has drawn the attention of the field due to its highly localized delivery of energy. This is because alpha particles have a short range and a higher linear energy transfer (LET) as compared with beta emitters. Understanding the temporal evolution and spatial dosimetry is essential to ensure the efficacy, safety, and feasibility of the treatment.

Typically, in vitro experiments targeting membrane-bound receptors work as a balance between the radiopharmaceutical binding of the receptors present on the membrane and the internalization process of the radiopharmaceutical penetrating the cytoplasm. Additionally, these processes compete with the dissociation of the radiopharmaceutical from the membrane and the excretion of the radiopharmaceutical from the cytoplasm to the cell culture medium.

We have developed a computational tool to model in vitro experiments with these features. Our tool simulates the time evolution of radioactive decay, including the entire decay chain of a given radionuclide.

Additionally, it considers the cell-washing procedures in which the activity in the medium or cell membrane can be removed. To model the pharmacokinetic of the experiment, a system of dynamic differential equations was implemented to control the spatial and temporal distribution of radiopharmaceuticals throughout the experiment. The decays are simulated into the cell medium, cell membrane, or cell cytoplasm following the mentioned RPTs distributions.

Our computational tool allows us to save the dose absorbed by each cell individually, with its temporal distribution. These options offer us a tool to perform time-structure microdosimetric studies. With our tool, two published experiments with PDAC and ES-2 cell lines were replicated, and our results were consistent with the findings reported in the articles.

Development of digital twins for calculating effective dose in humans exposed to high radiation.

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Abstract

Many radiation protection applications require the production of large numbers of accurate simulations of the interaction between radiation and the human body. This work implemented a Digital Twin System (DTS) to calculate the effective dose in humans exposed to environments with high radiation doses. Two approaches were used to generate anthropomorphic models: personalized phantom models that voxelized DICOM (Digital Imaging and Communications in Medicine) images from individuals and voxelized models of existing standard human phantoms according to ICRP110. With these capabilities, it is now possible to allow feedback and updating of the treatment plan with individual-specific information, offering a modular and adaptable solution, and increase precision due to the use of voxels, respectively. The new RadPhantom application, based on Monte Carlo methods, was developed to implement this DTS. This development integrates existing and publicly available models within MEIGA, a framework containing Geant4-based applications. This integration not only enables large-scale simulations in cloud-based environments, but also ensures reproducibility and adherence to the FAIR (Findable, Accessible, Interoperable, and Reusable) paradigm, using an integration of metadata and ontologies based on current standards. RadPhantom's functionality and efficiency were validated across diverse primary radiation types. Results consistently demonstrated accurate absorbed dose distributions and increasing effective doses with higher energy levels, aligning with regulatory recommendations. This work describes our implementation and provides some example results on human shielding materials and effective absorbed dose. Comparison with original phantom implementations showed no discrepancies in absorbed dose calculations and, by leveraging cloud-based resources and virtualized containers. RadPhantom completed simulations up to 25% faster than existing tools. These findings offer insights into the potential biological effects of simulated radiation scenarios, particularly in medical and aviation contexts. Moreover, RadPhantom can contribute to the evaluation of shielding materials in rapid-neutron production facilities and the evaluation of effective doses during severe accidents.

Spectral separation of laser-accelerated protons and ions in a magnetic dipole chicane

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Abstract

Ion acceleration by interactions of femtosecond laser pulses with thin targets has become a very active field of research. The particle energies typically follow an exponential distribution covering the entire interval up to a sharp maximum of several MeV. We have designed a magnetic dipole chicane for the spatial separation of protons with different momenta. It allows for the generation of quasi-monoenergetic proton beams at high-intensity laser facilities.

The particle beam released in the laser-plasma interaction passes through a collimator and two anti-parallel magnetic dipole fields generated by a series of identical C-magnets. The guidance of protons has been tested at the external beamline of the cyclotron at Centro Nacional de Aceleradores (CNA). The mechanical design of the outer support structure enables a flexible choice of the magnet positions and thereby the field configuration. The corresponding trajectories are simulated with a ray-tracing code. We have mounted a setup geometrically adapted to the vacuum chamber of the VEGA-3 laser (1 PW, 30 J) at Centro de Láseres Pulsados (CLPU). The separation of proton energies along the horizontal plane and their passage through a vacuum port have been demonstrated experimentally.

The energy selector has been applied in a radiobiology experiment at the VEGA-3 facility. It may be used in laser-proton acceleration up to about 12 MeV whenever a narrow particle spectrum at high peak fluence is of interest.

Financed by Generalitat Valenciana through the program “I+D+i Subvenciones para Grupos de investigación consolidados” (AICO), ref. CIAICO/2022/008, and CLPU, experiment 00562-0101. Supported by the Government of Castilla y León, ref. CLP263P20, co-financed with FEDER funds. M.C. Jiménez-Ramos acknowledges the support to this work through a VI PPIT-US contract.

Multiplexed physical sensing for cell detection and characterization

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Abstract

Cells are systems of exceptional interest not only for the wide knowledge they can provide about life and diseases, but also because the rich variety of physical phenomena that happen in them. Mechanics, electricity or molecular dynamics are some examples of different physical approaches under which the cell can be studied. Moreover, changes in one type of physical property can have an influence on other physical properties (e.g. changes in the molecular composition of the cell changes its mechanical, electrical or optical properties). Consequently, measuring physical properties of cells stands as a promising approach for performing label-free discerning between different types of cells as well as expanding our knowledge of different biological processes.

To this purpose, in this work we develop suspended microchannel resonators (SMR): a platform that allows a multiplexed physical characterization of single cells merging in a single device different physical sensing approaches (nanomechanics, microfluidics, optical scattering and dielectrophoresis). These devices consist on a microfluidic channel free-standing for a certain length so it can mechanically oscillate in flexural modes. By means of a laser doppler vibrometer and a piezoelectric actuator, the mechanical resonance frequency of this SMR device can be tracked, obtaining information about cell mass and hydrodynamics by analyzing the resonance frequency shifts individual cells produces as they pass through the free-standing zone.

Moreover, by integrating gold electrodes on the suspended microchannel, we have achieved complementing the cell mass sensing (obtained by the nanomechanical analysis) with electrical information of the sample. These electrodes, allow generating a non-uniform electric field inside the suspended microchannel, which not only opens the door to cell immobilization but also allows measuring some novel electro-thermo-mechanical effects in the device which can be used to obtain additional information about the medium in which the cells are suspended.

The utilisation of laser technology for the objective classification of the posture of individuals who are bedridden.

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Abstract

This paper presents an innovative method for the automated classification of postures of bedridden patients using laser technology. The objective is to improve the quality of medical care and facilitate the continuous monitoring of patients in clinical and home environments. A system is proposed that uses laser sensors to capture the three-dimensional geometry of body postures. A robust classification algorithm is developed using advanced computer vision processing techniques, capable of identifying and categorising lateral decubitus postures, also known as lateral safety positions. These are commonly used to position patients who are permanently bedridden. The experimental results thus far indicate that the technology has sufficient accuracy for posture classification, suggesting the potential for this technology to improve the monitoring and care of bedridden patients. Furthermore, it provides periodic warnings to medical staff

when a patient has exceeded the recommended time in the same posture, thus avoiding the occurrence of skin ulcers.

Grant PID2021-123948OB-I00 funded by MCIN/AEI/10.13039/501100011033 and by ERDF “A way of making Europe”, by the European Union. David S. Canzobre was financed by the Campus Industrial de Ferrol (Universidade da Coruña) through Industrial Doctorate Grants. The authors are grateful for the collaboration of Anta Norte S.L.

Film Dosimetry Based on a Multivariant Net Optical Density Approach

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Abstract

We present a new multichannel filtering approach for extracting and combining detailed dosimetric information from scanned radiochromic films, even when these films are damaged and/or affected by lateral manufacturing heterogeneities. To this aim, we make use of Bayesian inference techniques. Within this theoretical framework, the film dose map is estimated from the maximum of the posterior conditional probability distribution of the net optical density at each pixel. Since the prior net optical density distribution of pixel values for each channel (red, green, and blue) and dose is described by a multivariate Gaussian distribution, the most probable pixel dose is estimated as the maximum of the Gaussian fitting curve of the posterior net optical density. As demonstrated, this is a direct consequence of applying the central limit theorem to the collected transmitted photon distribution in each scanner pixel. In contrast to previous multi-Gaussian approaches, this new filter is formulated in terms of the net optical density distribution, which allows for linear net optical density dose factors. Gamma scores of EBT3 and EBT-XD film dosimetries for several real radiotherapy plans, after applying our multi-Gaussian filter, show remarkable results (more than 96.9% using a 2% dose difference and 2 mm distance-to-agreement difference criterion) when compared to theoretical plans from the Pinnacle Planning System. These scores overcome those obtained via other filters (Lewis et al., Méndez et al., or without multichannel filtering).

POSTER: Assessment of PRIMO-PenEasy Monte Carlo Simulation Against Dosimetric Findings for 6 MV Photon Beams in Small Fields

Presenter

Nataly Diaz Universidad Complutense de Madrid

Co-presenter

Jose Manuel Udias Universidad Complutense de Madrid

Abstract

Validating dosimetry for small fields in clinical plans requires specialized instrumentation to ensure accuracy and spatial resolution. This study proposes a solution using PRIMO-penEasy Monte Carlo (MC) simulations when direct measurements are impractical or yield inconsistent results due to challenges posed by small fields.

Three tools were employed: the Semiflex ionization chamber PTW model 31010 in a water-filled acrylic tank, EBT3 radiochromic films within solid water phantom layers, and PRIMO-PenEasy MC simulations for

small photon beams. Experimental dosimetric data were collected at San Ignacio University Hospital in Bogota, Colombia, involving two small fields and one conventional field generated by an Axesse-type linear accelerator.

Comparing radiochromic film EBT3 data to MC simulations revealed better agreement than with the ionization chamber, likely due to dose averaging across its detection volume. Variations in off-axis ratios were observed in both crossplane and inplane directions, particularly pronounced in small field configurations, possibly influenced by multi-blade collimation and XY-jaws.

The study demonstrated PRIMO-PenEasy MC simulation's ability to provide precise dose distributions for small photon beams from an Axesse-type linear accelerator. These simulation results reconcile disparities among measurements from different detectors, offering reliable indicators of accuracy for dosimetric validation in clinical plans.

POSTER: Radiomics for predicting individual Survival in Radiotherapy treatments

Presenter

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Co-presenters

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Abstract

We present a new and generic AI algorithm to predict the individualized survival of patients after radiotherapy treatment. We have developed an encoder-decoder model based on a Long-Short Term Memory (LSTM) recursive neural network. As input arguments, we use clinical attributes of each patient (age, gender, stage, etc.) as well as radiomic information at time t after treatment. Our model is trained by minimizing the mean square distance between the real individualized survival probability and the predicted one over time (Integrated Brier Score -IBS-). As a test, we made predictions on lung cancer patients belonging to the recent published data set Lung1 of the [NSCLC-Radiomics](#) study. Our model predicts a population survival curve compatible with that obtained by the Kaplan Maier estimator (classical statistics) and Random Survival Forest algorithm. Individualised survival probability predictions on validation data demonstrate the accuracy of our model ($IBS \sim 0.15$). Furthermore, our model is capable of assessing the relevance of variables with lower uncertainties compared to those obtained by the RSF.

POSTER: Evaluación de los factores que influyen en el registro de imágenes de perfusión obtenidas por láser Doppler, para el estudio de la microvascularización periférica

Presenter

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Abstract

INTRODUCCIÓN:

Los sistemas de imágenes por láser Doppler permiten evaluar la perfusión tisular sobre un área determinada en tiempo real y sin contacto, registrando las variaciones en la frecuencia de la luz láser en estructuras en movimiento, como los glóbulos rojos. En este trabajo se analizan los factores asociados al registro de la imagen de perfusión que pueden afectar a la medida realizada y por tanto a su reproducibilidad: distancia fotodetector-objeto, resolución y velocidad del escaneo, y ángulo de incidencia del láser sobre la superficie de medida.

METODOLOGIA

Equipo de medida: MOORLDI2-IR. El objeto utilizado para la realización de las experiencias ha sido el dispositivo suministrado por el fabricante para el calibrado del equipo (suspensión coloidal estandarizada de microesferas de poliestireno con movimiento browniano tras una agitación de 30 segundos y 3 minutos de espera)

RESULTADOS

Se realizaron 24 determinaciones de la perfusión del objeto analizado en tres días distintos y con tres resoluciones diferentes: 64x64, 128x128 y 256x256 píxeles. obteniéndose coeficientes de variación del 0,98%, 1,36% y 1,38%, respectivamente.

Se realizaron 30 determinaciones a dos velocidades de escaneo: 4 y 10 ms/píxel con variabilidades del 2,01% y 1,77%, respectivamente. La distancia equipo-objeto se varió de 30 a 50 cm en incrementos de 5 cm, sin una diferencia estadística significativa en la variación y el ángulo de incidencia se varió de 0º a 48 grados con incrementos de 5 grados, mostrando que un ángulo de 5º presentaba la mínima variabilidad, 3,7%.

CONCLUSIONES:

El sistema tiene una adecuada reproducibilidad de las medidas, la velocidad y resolución del escaneo afectan al tiempo de duración de la medida, factor importante al evaluar cambios fisiológicos de oclusión o hipo-hipertermia; 128x y 4ms reducen el tiempo de escaneo a la mitad y ofrecen buenos resultados y hasta 5 grados es un ángulo de incidencia óptimo.

Quantum Information (GEIC) / Información Cuántica (GEIC)

Organiser

Diego Porras

Invited speakers

Álvaro Alhambra (IFT-CDIC) Jara Juana Bermejo Vega (Universidad de Granada)

Symposium abstract

The symposium is organized by the Quantum Information and Computation Group (GEIC) of the RSEF. It is dedicated to: (i) Developments in quantum information theory (ii) Experimental and theoretical quantum computing: new quantum algorithms and their applications, progress in quantum computation architectures (superconducting qubits, trapped ions, photonic systems). (iii) Numerical methods for describing quantum computers, tensor networks and matrix product states, and quantum-inspired computational methods. Other quantum technologies are included in a separate symposium (Symposium on Quantum Technologies).

El simposio está organizado por el Grupo de Computación e Información Cuántica (GEIC) de la RSEF. Se dedica a: (i) Desarrollos en la teoría de la información cuántica. (ii) Computación cuántica experimental y teórica: nuevos algoritmos cuánticos y sus aplicaciones, avances en las arquitecturas de computación cuántica (qubits superconductores, iones atrapados, sistemas fotónicos). (iii) Métodos numéricos para describir computadoras cuánticas, redes tensoriales y estados de productos matriciales, y métodos computacionales de inspiración cuántica. Otras tecnologías cuánticas se incluyen en un simposio separado (Simposio sobre tecnologías cuánticas).

List of abstracts at the symposium

Efficient quantum Gibbs samplers

1st author

Alvaro Alhambra IFT-CSIC

Abstract

In quantum computing and simulation, one of our main goals is to efficiently mimic natural quantum phenomena in a controlled manner. The process of thermalization, or the preparation of thermal states of matter is one such crucial task. In this talk, we will introduce a recent efficiently implementable dissipative evolution that models thermalization, and prove that it is efficient in system size at high enough temperatures for any local Hamiltonian on a lattice. We will also show how the algorithm simplifies when the underlying model is commuting, in which case we can also prove stronger convergence guarantees. Finally, we show how our results also yield the efficient adiabatic preparation of the associated purifications or “thermofield double” states.

Dynamics of stochastic Hamiltonian: from control to chaos

1st author

Aurelia Chenu University of Luxembourg

Abstract

Quantum experiments are performed in noisy platforms. In NISQ devices, realistic setups can be described by open systems or noisy Hamiltonians. Starting from a generic noisy Hamiltonian, I will first present a scheme to simulate long-range and many-body interaction in a quantum platform [1]. The scheme is then

adapted to control the thermalization of a harmonic oscillator [2] and generate a squeezed thermal state [3] in arbitrary time.

Then, going beyond the noise-averaged density matrix, I will introduce the concept of stochastic operator variance (SOV) of an observable. The SOV [4] is an operator that characterizes the deviation of any operator from the noise-averaged operator in a stochastic evolution governed by the Hamiltonian. As such, it is relevant in the quantum simulation of open systems using NISQ devices, e.g., to engineer a given dissipative evolution. Surprisingly, we find that the evolution of the noise-averaged variance relates to an out-of-time-order correlator (OTOC), which connects fluctuations of the system with scrambling. This connection may allow computing the Lyapunov exponent and experimentally access OTOCs without the need to invert the sign of the Hamiltonian. I will illustrate the results in the stochastic LMG model, and show how noise changes the phase diagram of the system.

In the last part, I will present how the stochastic model is suited to explain the variance of the density matrix measured in a dissipative qubit.

[1] A. Chenu, M. Beau, J. Cao, and A. del Campo. Phys. Rev. Lett. 118:140403 (2017)

[2] L. Dupays, I. L. Egusquiza, A. del Campo, and A. Chenu. Superadiabatic thermalization of a quantum oscillator by engineered dephasing, Phys. Rev. Res. 2:033178 (2020)

[3] L. Dupays and A. Chenu. Dynamical engineering of squeezed thermal state, Quantum 5:449 (2021)

[4] P. Martinez-Azcona, A. Kundu, A. del Campo, and A. Chenu, Phys. Rev. Lett. 131:16202 (2023).

Study of quantum phase transitions in static systems through periodically quenched systems

1st author

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Abstract

Quantum phase transitions encompass a variety of phenomena that occur in quantum systems exhibiting several possible symmetries. Traditionally, these transitions are explored by continuously varying a control parameter that connects two different symmetry configurations. We propose an alternative that, by abruptly and periodically shifting between symmetry configurations, one may observe precursors of the quantum phase transition of the analogous static system that displays such symmetries. This approach allows the use of time as an effective control parameter which may prove experimentally useful in situations where accessing the traditional control parameter is challenging.

Shortcuts to Adiabaticity in Krylov Space

1st author

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Adolfo del Campo University of Luxembourg

Abstract

Shortcuts to adiabaticity provide fast protocols for quantum state preparation in which the use of auxiliary counterdiabatic controls circumvents the requirement of slow driving in adiabatic strategies. While their development is well established in simple systems, their engineering and implementation are challenging in many-body quantum systems with many degrees of freedom. We show that the equation for the counterdiabatic term, equivalently the adiabatic gauge potential, is solved by introducing a Krylov basis. The Krylov basis spans the minimal operator subspace in which the dynamics unfolds and provides an efficient way to construct the counterdiabatic term. We apply our strategy to paradigmatic single- and many-particle models. The properties of the counterdiabatic term are reflected in the Lanczos coefficients obtained in the course of the construction of the Krylov basis by an algorithmic method. We examine how the expansion in the Krylov basis incorporates many-body interactions in the counterdiabatic term.

Ref. Kazutaka Takahashi, Adolfo del Campo, Phys. Rev. X 14, 011032 (2024)

Simplifying the simulation of local Hamiltonian dynamics

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Abstract

Local Hamiltonians, H_k , describe non-trivial k -body interactions in quantum many-body systems. Here, we address the dynamical simulatability of a k -local Hamiltonian by a simpler one, $H_{k'}$, with $k' < k$, under the realistic constraint that both Hamiltonians act on the same Hilbert space. When it comes to exact simulation, we build upon known methods to derive examples of H_k and $H_{k'}$ that simulate the same physics. We also address the most realistic case of approximate simulation. There, we upper-bound the error up to which a Hamiltonian can simulate another one, regardless of their internal structure, and show an example suggesting that the accuracy of a $(k'=2)$ -local Hamiltonian to simulate $H_{k'}$ with $k > 2$ increases with k . Finally, we propose a method to search for the k' -local Hamiltonian that simulates, with the highest possible precision, the short time dynamics of a given H_k Hamiltonian.

Indistinguishability of identical bosons from a quantum information theory perspective

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Abstract

We present a general theory of indistinguishability of identical bosons in experiments consisting of passive linear optics followed by particle number detection. Our approach uses tools from quantum information theory and the results do neither rely on additional assumptions on the input state of the interferometer, such as fixed mode occupation number, nor on the degrees of freedom that potentially make the particles distinguishable. We identify the expectation value of the projector onto the N -particle symmetric subspace as an operationally meaningful measure of indistinguishability, and derive tight and efficiently measurable lower bounds. We present a definition of perfect distinguishability and characterize the corresponding set of states.

Quantum Reservoir Computing in ordered atomic lattices

1st author

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Roberta Zambrini IFISC: Instituto de Física Interdisciplinar y Sistemas Complejos

Abstract

Quantum reservoir computing (QRC) exploits the dynamical properties of quantum systems for machine learning tasks. Building upon classical reservoir computing, Fujii and Nakajima [1] showed the learning capabilities in temporal tasks of a quantum disordered Ising model. Since their seminal work, the field has rapidly evolved for the potential of exploiting the large Hilbert space of quantum states to process classical and quantum inputs data, as well as for fast and easy training. As shown in [2], the working dynamical regime of the reservoir is a fundamental factor in achieving high computational capabilities. Indeed, the ergodic phase is much more expressive than the many-body localization phase. While all the existing literature

about QRC is based on disordered systems, which are good candidates to work in the ergodic phase. In this work, we consider a reservoir made of a regular Bose-Hubbard chain in different (Mott-insulator and the superfluid) regimes. We show that disorder is not a necessary condition for QRC, which can facilitate future experiments on real quantum devices. Moreover, we provide strong evidence that optimal performance of the algorithm is achieved in a chaotic dynamical region that emerges for Hamiltonian parameters corresponding to the transition from the superfluid to the Mott insulator phase.

[1] K. Fujii and K. Nakajima. Harnessing disordered-ensemble quantum dynamics for machine learning. *Physical Review Applied*, 8(2):024030, 2017.

[2] R. Martínez-Peña, G. L. Giorgi, J. Nokkala, M. Soriano, and R. Zambrini. Dynamical phase transitions in quantum reservoir computing. *Physical Review Letters*, 127(10):100

Conditional photonic phase gate in topological waveguide QED

1st author

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Abstract

Topological photonics provides a route to engineer one-way and robust-to-disorder photon flows [1]. An open question in the field is whether it is possible to perform controlled quantum operations between these topologically protected photons, a challenging task due to their non-interacting character [2]. In this work, we provide a positive answer to this question by showing how to engineer a controlled phase gate between two photonic qubits propagating in orthogonal, topologically-protected edge channels appearing in two-dimensional photonic insulators [3]. The only ingredients required are the coupling of several two-level emitters to these channels and a suitable choice of the photonic qubit encoding such that the photons cross as they propagate through the emitters [4,5]. We study the fidelity of the conditional gate and its resilience to imperfections by calculating the single and two-photon scattering matrix of the system and demonstrate how it can achieve high fidelities with a moderate number of emitters. Our work paves the way for harnessing topological photonics systems for photonic quantum information processing.

[1] Tomoki Ozawa, Hannah M. Price, Alberto Amo, Nathan Goldman, Mohammad Hafezi, Ling Lu, Mikael C. Rechtsman, David Schuster, Jonathan Simon, Oded Zilberberg, and Iacopo Carusotto. Topological photonics. *Rev. Mod. Phys.*, 91(1):15006, Mar 2019.

[2] Darrick E. Chang, Vladan Vuletić, and Mikhail D. Lukin. Quantum nonlinear optics — photon by photon. *Nat. Photon.*, 8(9):685–694, Aug 2014.

[3] Carlos Vega, Diego Porras, and Alejandro González-Tudela. Topological multimode waveguide QED. *Phys. Rev. Res.*, 5(2):023031, Apr 2023.

[4] Daniel J. Brod and Joshua Combes. Passive CPHASE Gate via Cross-Kerr Nonlinearities. *Phys. Rev. Lett.*, 117(8):080502, Aug 2016.

[5] Björn Schränski, Miren Lemaître, and Anders S. Sørensen. Passive Quantum Phase Gate for Photons Based on Three Level Emitters. *Phys. Rev. Lett.*, 129(13):130502, Sep 2022.

Hole Flying Qubits in Quantum Dot Arrays

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Abstract

Recent advancements in semiconductor Quantum Dot Arrays (QDAs) have propelled the field towards greater scalability, unlocking applications in quantum computation, information processing, and simulation [1-3]. Notably, hole spin qubits have garnered attention for their minimal hyperfine interaction and intrinsic Spin-Orbit Interaction (SOI) [4].

This study investigates QDAs as quantum links, facilitating information transfer between distant dots. Despite the increasing popularity of long-range transfer protocols, the advantages of SOI in QDAs are largely untapped. We propose a novel method employing Shortcuts to Adiabaticity (STA) to implement hole-flying qubits in QDAs.

Our investigation demonstrates the tunability of hole spin rotation during transfer by adjusting the number of dots and SOI via external electric fields. This tunability controls the rotated angle and modulates the rotation vector. By employing a sequence of up to three long-range transfers, we simultaneously implement a general one-qubit gate, accelerating quantum entanglement generation between distant sites. Furthermore, we propose strategies to mitigate dephasing effects, integrating dynamical decoupling protocols during the transfer process. These findings extend to systems with multiple interacting particles, enabling long-range quantum entanglement distribution. Additionally, we demonstrate long-range spin

transfer in half-filled QDAs, leveraging SOI in combination with high magnetic fields to establish dark states that prevent the population of intermediate states.

Our study advances the understanding of long-range transfer in QDAs, addressing critical aspects for practical quantum computation. We propose QDAs to overcome scalability issues, employing them as quantum links to interconnect computing nodes.

- [1] S. G. J. Philips, et al., Nature 609, 919 (2022).
- [2] I. Seidler, et al., npj Quantum Inf 8, 100 (2022).
- [3] A. Zwerver, et al., PRX Quantum 4, 030303 (2023).
- [4] N. W. Hendrickx, et al., Nature 591, 580 (2021).
- [5] D. Fernández-Fernández, arXiv: 2312.04631 (2023).
- [6] Y. Ban, et al., Nanotech. 29, 505201 (2018).

Resilient multi-mode superconducting qubit designed with evolutionary algorithms

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Abstract

Multi-mode superconducting circuits offer a highly promising platform for engineering robust systems for quantum computation. However, as the system's dimensionality increases beyond the usual single-mode, its design and study become exponentially complicated and less intuitive. Previous studies of single-mode devices have demonstrated that superconducting quantum systems can be engineered to be robust against various sources of noise and decoherence. Nevertheless, advancements in single-mode device design have revealed that no device with a single degree of freedom can be engineered to be simultaneously resilient to multiple sources of decoherence, as the necessary protection requirements often conflict. This observation highlights the need to explore systems with a larger number of degrees of freedom, which have proven effective in providing protection against different error sources simultaneously. Unfortunately, this protection typically comes with construction constraints (such as symmetry requirements) and limitations in manipulability.

In this study, we present novel multi-mode qubit architectures designed using evolutionary algorithms that exhibit desirable qubit characteristics, including restricted transitions, improved relaxation and dephasing times, and resilience against fabrication defects. The additional degrees of freedom offered by the multi-mode structure are utilized to mitigate noise sensitivity. We explore heterogeneous configurations where different parts of the system are suitable for specific operations, such as readout or control. This approach is valuable for identifying configurations that, although lacking the complete protection of symmetry-protected systems, strike a balance between manipulability, construction, and noise protection. Furthermore, we analyze how the generated systems respond to fluctuations in parameter values caused by fabrication errors, which is crucial for practical implementation.

Reliable quantum computational advantages from quantum simulation

1st author

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Abstract

Demonstrating quantum advantages in near term quantum devices is a notoriously difficult task. Ongoing efforts try to overcome different limitations of quantum devices without fault-tolerance, such as their limited system size or obstacles towards verification of the outcome of the computation. Proposals that exhibit more reliable quantum advantages for classically hard-to-simulate verifiable problems lack, at the same time, practical applicability. In this talk we will review different approaches to demonstrate quantum advantages inspired from many-body quantum physics. The first of them use entangled quantum resources such as cluster states, which are useful to demonstrate verifiable quantum advantages based on sampling problems (Theory proposal J. Bermejo-Vega, et al. Phys. Rev. X 8, 021010, 2018 and recent experimental demonstration arXiv preprint arXiv:2307.14424). The second probe measurement of many-body quantities such as dynamical structure factors in quantum simulation setups (Dynamical structure factors of dynamical quantum simulators, ML Baez, M Goihl, J Haferkamp, J Bermejo-Vega, M Gluza, J Eisert, Proceedings of the National Academy of Sciences 117 (42), 26123-26134).

The Bethe ansatz as a quantum circuit

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Abstract

The Bethe ansatz represents an analytical method enabling the exact solution of numerous models in condensed matter physics and statistical mechanics. When a global symmetry is present, the trial wavefunctions of the Bethe ansatz consist of plane wave superpositions. It has been shown that the Bethe ansatz can be recast as a deterministic quantum circuit. Here we derive the analytic form of the circuit gates, which was previously lacking. As a crucial step, we present a simple set of diagrammatic rules that define a Matrix Product State building Bethe wavefunctions. Remarkably, this provides a new perspective on the equivalence between the coordinate and algebraic versions of the Bethe ansatz. We illustrate our method on the spin-1/2 XX and XXZ models. We show that using this approach one can efficiently prepare eigenstates of the XX model on a quantum computer with quantum resources that match previous state-of-the-art approaches.

Solving Non-Unitary Dynamics on Digital Quantum Computers: Quantum Imaginary Time Evolution (QITE)

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Abstract

Quantum Imaginary Time Evolution (QITE) is a powerful algorithm designed to simulate the non-unitary dynamics of quantum systems on quantum computing architectures. QITE efficiently leverages quantum parallelism to find ground states by approximating non-unitary evolution with unitary operations. The QITE process involves discretizing imaginary time evolution, applying Trotter decomposition, and implementing unitary operations, making it scalable and practical for complex quantum systems. All quantum gates in quantum computing are inherently unitary, making QITE essential for simulating non-unitary dynamics on quantum hardware. Non-unitary dynamics, critical for understanding out-of-equilibrium processes, cannot be accurately described by the Schrödinger equation, necessitating approaches like QITE. The Glauber Ising model exemplifies such dynamics, where spins flip according to probabilistic rules influenced by local fields. This model is essential for studying systems influenced by their environment, providing insights into how external factors affect system behavior. By applying QITE, we can effectively study these non-equilibrium systems, providing insights into their behavior

Error estimation in current noisy quantum computers

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Abstract

One of the main important features of the noisy intermediate-scale quantum (NISQ) era is the correct evaluation and consideration of errors. In this paper, we analyze the main sources of errors in current (IBM) quantum computers and we present a useful tool (TED-qc) designed to facilitate the total error probability expected for any quantum circuit. We propose this total error probability as the best way to estimate a lower bound for the fidelity in the NISQ era, avoiding the necessity of comparing the quantum calculations with any classical one. In order to contrast the robustness of

our tool we compute the total error probability that may occur in three different quantum models: 1) the Ising model, 2) the Quantum-Phase Estimation (QPE), and 3) the Grover's algorithm. For each model, the main quantities of interest are computed and benchmarked against the reference simulator's results as a function of the error probability for a representative and statistically significant sample size. The analysis is satisfactory in more than the 99% of the cases. In addition, we study how error mitigation techniques are able to eliminate the noise induced during the measurement.

Characterizing convergence speed of dissipative ground state preparation algorithms

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Abstract

Ground state preparation is a fundamental problem in physics, which stands challenging even for quantum computers. In the context of near-term devices, dissipative preparation methods have gained attention due to their resilience to noise. These methods imitate natural energy dissipation utilizing partial measurements and conditioned operations to gradually prepare the desired state. Although they stand out as a promising approach for NISQ devices, analyzing their performance presents a unique set of challenges.

As previous research in quantum channels has primarily focused on determining the impact of noise, it has often neglected pure state fixed points and characterizing convergence speed - crucial aspects for quantum algorithms. In this presentation, we redirect the interest focus by introducing mathematical techniques for analyzing the distance between the target and prepared states and the convergence speed. We apply them in the context of channel composition, which naturally arises in algorithms implemented as the iteration over a dissipative subroutine. Our techniques also present applications as new characterizations of the impact of quantum noise.

Towards scalable implementations of digital-analog quantum computing

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Abstract

Digital-analog quantum computing (DAQC) is a computational paradigm which employs an analog Hamiltonian resource together with single-qubit gates to reach universality [1]. This protocol benefits from the natural interaction Hamiltonian of quantum systems, as instead of trying to eliminate it enables us to use it as a resource. Additionally, it has been shown that this paradigm has inherent error mitigation capabilities. Since it only requires the application of single qubit gates, it avoids the use of the noisier two qubit gates, providing a promising way of implementing algorithms in the NISQ era.

Regarding its applicability, it has already been shown useful for implementing ubiquitous quantum algorithms and solving various problems. Among them, the quantum Fourier Transform, the algorithm for solving a linear system of equations (HHL) or a simulation of fermionic systems.

In this talk, we will focus on two new recent works that advance the state-of-the-art of DAQC.

First, we propose a new protocol to simulate arbitrary two-body Hamiltonians. We showed that the simulation of an arbitrary two-body target Hamiltonian of n qubits requires $O(n^2)$ analog blocks with guaranteed positive times, providing a polynomial advantage compared to the previous schemes [2].

Second, we focus on the stability of DAQC in a noisy environment. Previously, it was shown that DAQC provided better resilience against both incoherent (dephasing and decoherence) and coherent errors (deviations on single qubit gate angles). Now, we study the effect of misscalibration of the system, in particular, errors in the measurement of the couplings in the system. We show that DAQC is stable when measuring local observables for quantum simulation tasks. This allows us to show that the errors don't grow with the system size [3].

Both results contribute to showing the feasibility of scaling DAQC implementations to a higher number of qubits.

[1] A. Parra-Rodriguez, Phys. Rev. A 101, 022305 (2020)

[2] M. Garcia-de-Andoin, et al. Phys. Rev. Research 6, 013280 (2024)

[3] A. Álvares, et al. In preparation

Quantum reservoir computing complexity by a Krylov evolution approach

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Abstract

Quantum reservoir computing algorithms recently emerged as a standout approach in the development of successful methods for the NISQ era, because of its superb performance and compatibility with current quantum devices. By harnessing the properties and dynamics of a quantum system, quantum reservoir computing effectively uncovers hidden patterns in data. However, the design of the quantum reservoir is crucial to this end, in order to ensure an optimal performance of the algorithm.

In this work, we introduce a precise quantitative method, with strong physical foundations based on the Krylov evolution, to assess the wanted good performance in machine learning tasks. Our results show that the Krylov approach to complexity strongly correlates with quantum reservoir performance, making it a powerful tool in the quest for optimally designed quantum reservoirs, which will pave the road to the implementation of successful quantum machine learning methods.

Gradients and frequency profiles of quantum re-uploading models

1st author

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Abstract

Quantum re-uploading models have been extensively investigated as a form of machine learning within the context of variational quantum algorithms. Although theoretically universal, their trainability and expressivity are critical to their performance and not yet fully understood. In this work, we address trainability through the lens of the magnitude of the gradients of the cost function. We prove bounds for the differences between gradients of the better-studied data-less parameterized quantum circuits and re-uploading models. We coin the concept of absorption witness to quantify such difference. For the expressivity, we prove that quantum re-uploading models output functions with vanishing high-frequency components and upper-bounded derivatives with respect to data. As a consequence, such functions

present limited sensitivity to fine details, which protects against overfitting. We performed numerical experiments extending the theoretical results to more relaxed and realistic conditions. Overall, future designs of quantum re-uploading models will benefit from the strengthened knowledge delivered by the uncovering of absorption witnesses and vanishing high frequencies.

Quantum statistical inference techniques for sensing and metrology

1st author

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Abstract

Quantum sensing and metrology exploits uniquely quantum features for the design of sensors and protocols that surpass their classical analogues. In many instances, the key resource in such protocols is entanglement which is often costly to prepare and maintain. Moreover, there are important sensing and metrological scenarios where entanglement may not even be available---such as in imaging of distant point sources, or bio photons. In these cases the advantages of quantum sensors are derived by clever design of the measurements. In this talk I will review a variety of sensing and metrological paradigms where entanglement among the probes is absent and use quantum statistical inference techniques to derive optimal measurement schemes that furnish increased precision.

Quantum reservoir computing in finite dimensions

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Abstract

Quantum reservoir computing (QRC) is a machine learning technique where complex quantum systems are exploited to solve temporal tasks, such as predicting chaotic time series and complex spatiotemporal dynamics. Most existing results in the analysis of QRC systems with classical inputs have been obtained using the density matrix formalism. Our work shows that alternative representations can provide better insights when dealing with design and assessment questions. It has been shown that these vector representations yield state-affine systems (SAS) previously introduced in the classical reservoir computing literature and for which numerous theoretical results have been established. This connection has been used to show that various statements in relation to the fading memory (FMP) and the echo state (ESP) properties are independent of the representation, and also to shed some light on fundamental questions in QRC theory in finite dimensions. Our conclusions can be summarised as: the necessary and sufficient condition that makes a quantum reservoir valuable is strictly contractive dynamics towards input-dependent fixed points.

Quantum Time-series Learning with Evolutionary Algorithms

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Abstract

In the current NISQ scenario of quantum computing, variational methods have arisen as strong candidates. These methods require the optimization of many parameters, a task most typically tackled through gradient-based techniques such as Adam and RMSprop. However, it is known that several difficulties appear in this optimization such as local minima. Evolutionary algorithms, loosely inspired by biological evolution, are a kind of global search that probes the search space in an inherently different way, through spread, recombination and selection of parameter values. Time-series forecast is a task where one aims to predict the future steps of sequential data with knowledge of past data.

In this work, we present a method to use evolutionary algorithms to optimize parameters on a quantum circuit dedicated to making predictions on a time series. We observe that the choice of evolutionary algorithms greatly affects performance, and one such algorithm -- the covariant-matrix adaptation evolutionary strategy (CMA-ES) -- stands out as most effective.

With CMA-ES, we perform a comparison between evolutionary and gradient-based parameter optimization for diverse instances of real-world data. We find that, although gradient-based methods are typically faster, they typically get trapped in local minima from which no reasonable amount of further training can remove them. On the other hand, evolutionary algorithms applied to the same dataset are able to avoid such local minima, in what amounts to a five-fold decrease in prediction error for all tested datasets. Finally, the combined use of evolutionary and gradient-based methods is explored, and the results indicate it can be tuned to retain the advantages of both. The use of such combined strategies has the potential to enhance performance for variational algorithms, especially those sensitive to gains in accuracy.

POSTER: New Scientific Method, based on Natural/Universal Intelligence.

Presenter

José Daniel Sierra Murillo Universidad de La Rioja

Abstract

In this article, author intends to propose a New Scientific Method based on what he is going to call Natural/Universal Intelligence. Built on the enormous amount of information stored on the *Internet* and all the information storage and management systems connected to the Network of Networks. [1,2] The methodology used in the aforementioned construction of said New Scientific Method will consist of the structured and adequately planned management of all this enormous amount of information, through programming aimed at establishing general patterns of behavior/functioning of Nature/Universe. When talking about Artificial Intelligence (AI), reference is made to programming, manipulation and control, using an artificial language similar to traditional programming languages (Basic, Fortran, C, etc.) and other more recent ones. creation (Phyton for example), of various systems that flood our technological world today. "*Nothing new under the Sun*". [3,4] However, author believes that the step to take to a new paradigm is to know how to constructively use our Intelligence and use the Natural Reality that surrounds us and we know, together with the Reality of the Universe (or Universes) that we know today, knowledge that we can expand with a new Construction Tool based on Real Intelligence: Natural and Universal. Can we do it now?

[1] Bianchini, S., Müller, M., Pelletier, P., "Artificial intelligence in science: An emerging general method of invention", *Res. Policy*, 2022, ISSN 0048-7333 Vol. 51, Nº 10, pp. 104604 (1-15). <https://doi.org/10.1016/j.respol.2022.104604>.

[2] Alberto Suárez González, *Encuentros multidisciplinares*, 2014, ISSN-e 1139-9325, Vol. 16, Nº 47, pp. 1-10.

[3] Alan M. Turing, "Computing machinery and intelligence". *Mind*, 1950, Vol. 59, Nº 236, pp. 433-460.

[4] Brian Randell, "From Analytical Engine to Electronic Digital Computer: The Contributions of Ludgate, Torres, and Bush". *IEEE Annals of the History of Computing*, 1982, Vol. 4, Nº 4, pp. 327-341.

POSTER: On the existence of unbiased resilient estimators in discrete quantum systems

Presenter

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Abstract

Cramér-Rao constitutes a crucial lower bound for the mean squared error of an estimator in frequentist parameter estimation, albeit paradoxically demanding highly accurate prior knowledge of the parameter to be estimated. Indeed, this information is usually needed to construct the optimal unbiased estimator, which is highly dependent on the parameter. Conversely, Bhattacharyya bounds result in a more resilient estimation of prior accuracy by imposing additional constraints on the estimator. Initially, we conduct a quantitative comparison of the performance between Cramér-Rao and Bhattacharyya bounds when faced with less-than-ideal prior knowledge of the parameter. Furthermore, we demonstrate that the n th-order classical and quantum Bhattacharyya bounds cannot be computed –given the absence of estimators satisfying the constraints– under specific conditions tied to the dimension m of the discrete system. Intriguingly, for a system with the same dimension “ m ”, the maximum non-trivial order n is $m - 1$ in the classical case, while in the quantum realm, it extends to $m(m+1)/2 - 1$. Consequently, for a given system dimension, one can construct estimators in quantum systems that exhibit increased robustness to prior ignorance.

POSTER: Solving the Jaynes-Cummings Hamiltonian in an IBM quantum computer

Presenter

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Abstract

Quantum simulations are an attractive pathway to simulate complex quantum effects in physical systems in condensed matter [1], quantum chemistry [2], and high-energy physics [3], for example. Here we consider the interaction of optical nanoantennas with quantum emitters, which has applications such as enhancing the spectroscopic signal for molecular characterization and enabling faster single photon sources. This emitter-nanoantenna coupling is often described by the Jaynes-Cummings Hamiltonian (JCH), but the extension of this description to systems involving many molecules becomes very demanding for classical computers.

As a first step, we solve the time dynamics of the JCH for one molecule coupled to a plasmonic mode. We first construct the quantum circuit that implements the unitary evolution of this Hamiltonian into the basis of Pauli operators. With this purpose, we map the bosonic plasmon operator into a collection of qubits that maintain the necessary commutation relation [4]. Interestingly, the simulations of the resonant system indicate that there is no trotterization error when the terms of the Hamiltonian are placed in order, which

enables a more efficient simulation due to the reduction of the noise. We obtain the population dynamics of the plasmonic nanoantenna and the quantum emitter using an IBM quantum computer, and we observe the Rabi oscillations that are one of the main characteristics of the time evolution of the JCH. To verify the validity of the quantum simulations, we compare these results with those obtained by classical simulations. We find a generally good agreement between these results, and further improvements will be considered to diminish the level of noise.

- [1] Wu, et.al. (2002). *Physical Review Letters*, 89(5), 057904.
- [2] Aspuru-Guzik, et. al. (2005). *Science*, 309(5741), 1704-1707.
- [3] Jordan, et.al. (2012). *Science*, 336(6085), 1130-1133.
- [4] Somma, (2005). *arXiv preprint quant-ph/0512209*.



Complex Systems / Sistemas Complejos (Grupo GEFENOL)

Organiser

Rosa M^a Benito (UPM), Enrique Abad (U. Extremadura), Pablo Hurtado (U. Granada), Juan José Mazo (UCM), Raúl Toral (IFISC-CSIC)

Invited speakers

Jose J. Ramasco (IFISC, CSIC - Universitat Illes Balears) Diego Maza (Universidad de Navarra) Inmaculada Leyva (Universidad Rey Juan Carlos) Chantal Valeriani (universidad Complutense de Madrid)

Abstract

Complex systems are typically characterized by a large number of constituents that interact with each other, giving rise to emergent behavior that cannot be explained solely from their individual properties ("the whole is more than the sum of the parts"). In this context, the intrinsic nonlinearity of the interactions plays an essential role. Despite the diversity of areas in which complexity emerges, there is a common approach based on statistical, nonlinear and computational physics. This symposium is dedicated to theory, study methodology, and applications around complexity. A non-exhaustive list of systems and phenomena of interest includes disordered systems, social and economic phenomena, epidemic models, stochastic transport phenomena, climatic phenomena, and neural, genetic and proteomic networks, among many others. Some of the techniques commonly employed are models in terms of probability distributions for different quantities of interest, Monte Carlo simulations, molecular dynamics, representations based on complex networks, and Big Data analysis relying on machine learning and AI algorithms.

Los sistemas complejos típicamente se caracterizan por un gran número de constituyentes que interaccionan entre sí, dando lugar a un comportamiento emergente que no puede explicarse únicamente a partir de las propiedades individuales de los mismos ("el todo es más que la suma de las partes"). En este contexto, la no linealidad intrínseca de las interacciones juega un papel esencial. A pesar de la diversidad de ámbitos en los que emerge la complejidad, existe un enfoque común basado en la física estadística, no lineal y computacional. El presente simposio está dedicado a teoría, metodología de estudio, y aplicaciones en torno a la complejidad. Una lista no exhaustiva de sistemas y fenómenos de interés incluye sistemas desordenados, fenómenos sociales y económicos, modelos epidémicos, fenómenos de transporte estocástico, fenómenos climáticos, y redes neuronales, genéticas y proteómicas, entre otros muchos. Algunas de las técnicas comúnmente empleadas son modelos en términos de distribuciones de probabilidad para distintas cantidades de interés, simulaciones de Monte Carlo, dinámica molecular, representaciones basadas en redes complejas, y análisis de Big Data mediante el uso de aprendizaje automático y algoritmos de inteligencia artificial.

List of abstracts at the symposium

Field theory for human mobility

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Abstract

Understanding human mobility is crucial for applications such as forecasting epidemics spreading, planning transport infrastructure and urbanism in general. While, traditionally, mobility information has been collected via surveys, the pervasive adoption of mobile technologies has brought a wealth of (real time) data. The easy access to this information opens the door to study theoretical questions so far unexplored. In this work, we show for a series of worldwide cities that commuting daily flows can be mapped into a well behaved vector field, fulfilling the divergence theorem and which is, besides, irrotational. This property allows us to define a potential for the field that can become a major instrument to determine separate

mobility basins and discern contiguous urban areas. We also show that empirical fluxes and potentials can be well reproduced and analytically characterized using the so-called gravity model, while other models based on intervening opportunities have serious difficulties. Furthermore, we explore the possibility of generalizing these results to all sorts of mobility, not only recurrent mobility, and find with a series of models the basic ingredients needed to have a field.

Humans versus Bots in debates about ecological sustainability on X

1st author

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Abstract

Environmental sustainability is one of the most relevant concerns of our time, affecting the entire planet and requiring coordinated global efforts. Our research examines the environmental sustainability discussions of humans and bots, comparing them with each other [1]. The social network X (formerly known as Twitter) can provide much information about the social perception on a multitude of topics, both because of its volume of users and because accessing it is easy and rapid. This makes it possible to study users' opinions on relevant issues, such as environmental sustainability. In [1], we give more extension to the research of [2] and [3], developing a bot identification model based on both the characteristics of the user's profile and the identification of behaviour patterns in interactions (tweet, retweet, reply and quote). In the same way as [2] to characterise the activity of each user, the type of message sent and its moment of occurrence in time were considered, constructing from this information a string of characters describing his/her behaviour. As expected, we found a number of bots, ranging 9-15% of the users of the network [4]. Additionally, comparing humans and bots, we carried out a study on global sentiment on environmental sustainability from 2006 to 2022, detecting a majority of positive tweets. In particular, higher radicalization was observed in tweets from bots during 4 months of 2022, but these messages continued to show positive sentiment. Finally, we carried out a lexical analysis of the tweets using network theory, finding some similarities between the words used by bots and humans.

[1] Mouronte-López, M. L., Gómez Sánchez-Seco, J., & Benito, R. M. (2024). Patterns of human and bots behaviour on Twitter conversations about sustainability. *Scientific Reports*, 14(1). <https://doi.org/10.1038/s41598-024-52471-z>

[2] Pasricha, N., & Hayes, C. (2019). Detecting Bot Behaviour in Social Media using Digital DNA Compression. *Irish Conference on Artificial Intelligence and Cognitive Science*. <https://www.semanticscholar.org/paper/Detecting-Bot-Behaviour-in-Social-Media-using-DNA-Pasricha-Hayes/7f88a79589f980baae72b4e0a627d85fb0aa6e66>

[3] Yang, C., Harkreader, R.C., & Gu, G. (2011). Empirical Evaluation and New Design for Fighting Evolving Twitter Spammers. *IEEE Transactions on Information Forensics and Security*, 8, 1280-1293. <https://doi.org/10.1109/TIFS.2013.2267732>

[4] Varol, O., Ferrara, E., Davis, C., Menczer, F., & Flammini, A. (2017). Online Human-Bot Interactions: Detection, Estimation, and Characterization. *Proceedings of the International AAAI Conference on Web and Social Media*, 11(1), 280-289. <https://doi.org/10.1609/icwsm.v11i1.14871>

Complex networks for ecosystem services

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Abstract

Managing ecosystems to sustain ecosystem services amidst global change presents a significant challenge for both scientists and policymakers. Predicting how various management strategies and changing conditions will affect ecosystem services is made challenging by the complex interactions within ecological and socioeconomic systems. Overlooking these interactions can result in missed opportunities to optimize ecosystem services. Essentially, this involves enhancing the health, productivity, or value of ecosystems for humans and other species. Given the nature of these interactions, network theory provides an optimal method for exploring their complexities. However, there has been limited research on how to effectively implement network analyses for ecosystem services management and research. This study aimed to review the main scientific literature investigating ecosystem services using network theory. We systematically selected studies that combine complex network analysis with ecosystem service research. A total of 130 published papers were analyzed to investigate their temporal and spatial distributions, spatial scales, topics of study, network metrics, and the types of network models used in case studies. Through this analysis, we aim to highlight how ecosystems and their services are modeled and analyzed, identifying methods that could potentially advance the research field. The findings reveal that research tends to rely on a limited set of network metrics and models. Therefore, there are ample opportunities to set future work directions and we concluded our work by outlining some of them.

Endemic infectious states below the epidemic threshold and beyond herd immunity

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Abstract

Epidemic spreading is a complex process involving multiple spacial scales: While the transmission of viruses occurs through close contact among individuals within a few meters, this process is intricately linked to human mobility, which spans distances ranging from a few to thousands of kilometers. We propose that the interplay between these different scales is the cause of the anomalous fade-outs characterized by low but persistent outbreaks observed during the recent COVID-19 pandemic, which hindered epidemic control and challenged classical modeling approaches.

Our proposed mechanism, encoded in a mathematical model, explicitly addresses the scales within cities by using a Susceptible-Infected-Recovered model within a metapopulation framework. However, our model

only provides a minimal depiction of larger scales through a small influx of infected individuals to account for undetected imported cases. Our methods rely on simulating this model, understanding the outcomes through a new analytical technique that means the coarse-graining of the local dynamics, and subsequently comparing our findings with data on the spread of COVID-19 in England.

Focusing on a regime where the external import of new infections is so small that cannot be detected from the analysis of epidemic curves, we find that outbreaks of finite duration percolate in time, resulting in overall low but long-living epidemic states. We also demonstrate that our model is able to reproduce some critical signatures observed in COVID-19 spreading. Overall, our findings defy our understanding of the concept of epidemic threshold and its relationship with outbreaks survival for disease control.

Ref.: Aguilar, J., García, B. A., Toral, R., Meloni, S., & Ramasco, J. J. (2023). Endemic infectious states below the epidemic threshold and beyond herd immunity. *Communications Physics*, 6(1), 187.

Fundamental challenges in applying Physics to the modelling of social phenomena

1st author

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Abstract

In recent years, the mathematical and computational modelling of social phenomena has risen to become a relevant transdisciplinary area, spanning from the Physics of Complex Systems to Computational Economics. However, many objections have been made to the general enterprise of formalizing social behaviour.

In this work, we primarily focus on analysing some of the most important arguments in this direction, from methodological to epistemological ones. We will see that many of these stem from contemporary research in Philosophy of Science, and have reached scientific practice in a limited fashion, for a variety of reasons. We do this with a critical emphasis on the arguments' validity and limitations, taking into account present and foreseeable challenges for the social sciences.

We will also argue in favour of incorporating different academic perspectives to conceptualize the modelling of social phenomena, such as the ones given by Mathematical Logic-driven disciplines like Computational Social Choice or Epistemic Game Theory, which deal with some of the aforementioned problems.

Fenómenos colectivos inducidos por fricción / Collective phenomena induced by friction

1st author

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Abstract

Los sistemas granulares son agregados muy grandes de partículas o “granos” que interactúan básicamente por contacto. Dado que estos contactos son intrínsecamente disipativos, el control y manejo de este tipo de materiales requiere de una inyección constante de energía, como, por ejemplo, cuando se espera que fluyan por cierta región del espacio. Por otra parte, y aunque pueda parecer que las fuerzas de fricción responsables de esta disipación se conocen en profundidad, las escalas y parámetros que controlan la disipación de energía no se conocen en profundidad lo que ocasiona por ejemplo, que la práctica total de los sistemas que transportan y dosifican este tipo de materiales estén sobredimensionados en lo que a inyección de energía se refiere. En esta charla comentaremos de forma general algunas de estas escalas y

mostraremos como, haciendo uso de una estrategia originalmente introducida para el transporte “ratchet”, es posible alcanzar un grado de control relevante sobre sistemas particulados, pudiendo inducir separación de fases granulares, convección, compactación y dosificación, entre otros comportamientos colectivos. Granular systems are very large aggregates of particles or “grains” that interact basically by contact. Since these contacts are inherently dissipative, the control and handling of these materials requires a constant injection of energy, such as when they are expected to flow through a certain region of space. On the other hand, and although it may seem that the friction forces responsible for this dissipation are known in depth, the scales and parameters that control energy dissipation are not well understood, which causes, for example, that the total practice of systems that transport and dose this type of materials are oversized in terms of energy injection. In this talk we will discuss in a general way some of these scales and we will show how, using a strategy originally introduced for “ratchet” transport, it is possible to achieve a relevant degree of control over particulate systems, being able to induce granular phase separation, convection, compaction and dosing.

Stability of a homonegeous state in a two-dimensional fluid of active rotors

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Abstract

We consider a fluid of hard disks which undergo a permanent rotation due to the presence of a systematic constant torque. As a consequence of particle collisions, deviations from the average spin occur in the fluid. We write down the corresponding hydrodynamic equations for this kind of fluid (in the constant transport coefficient approximation), which need to account for angular momentum balance. Additionally, and as a consequence of the active torque on the constituting particles, new contributions to the stress tensor emerge, including an antisymmetric component. We discuss on the structure of these balance equations and the new transport coefficients, and deduce the linear stability of a base state that is homogeneous and hydrostatic (density and temperature fields are constant and there is no flow velocity).

Surprisingly, we show that for wide ranges of the relevant parameter space, the homogeneous state is unstable, potentially giving rise to density unbalance and hence phase separation.

We discuss on the analogies of this phase separation induced by active rotation, in comparison with the motility-induced phase separation that is well known in active matter.

For the sake of illustration, we show some cases from simulation data.

Structural dynamics of metallic glass-formers

1st author

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Abstract

The atomic mobility and structural dynamics of disordered materials is a main topic in the study of complex systems. During the cooling of liquids towards the glass transition the particle dynamics becomes increasingly cooperative and rises orders of magnitude in timescale, from microseconds in the supercooled liquid to minutes, hours or even longer in the glass. The evolution of the relaxation timescale is also accompanied by modifications of the relaxation spectrum, which have large influences on the properties of the emerging, non-equilibrium glass state. In the glass, the structure is not frozen but it continuously evolves through slow structural changes by the process known as physical aging. Despite large efforts in modelling all these phenomena, the long timescales of the structural dynamics near the glass transition prevent direct comparison with simulations.

Disordered metals, liquids and glasses, offer a model system to study how the structural dynamics evolve through temperature and pressure. The non-directional nature of the metallic bonding results in a rather simple interaction between the constituent particles. In terms of the interatomic potential, they can be regarded as the real materials which most resemble a Lennard-Jones simulation. Therefore, metallic glass-formers provide a unique system, with simple interatomic potential, to explore the complex cooperative dynamics emerging in the glass state. We will present in this conference our recent explorations in metallic glass-formers [1,2,3] by means of mechanical relaxation tests and X-ray Photon Correlation Spectroscopy using coherent synchrotron light. The two techniques allow us to obtain both macroscopic and microscopic insight of the structural dynamics, being able to experimentally resolve the Intermediate Scattering Function at the atomic length scale and relate it with dynamic properties like viscosity and relaxation modulus.

[1] Physical Review Letters 129, 175501 (2022)

[2] Nature Communications 14, 8407 (2023)

[3] Physical Review Letters 132, 056101 (2024)

Electrothermoplasmonic Flow In Gold Nanoparticle Suspensions

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Abstract

Efficient mixing and pumping of liquids at the microscale is a technology that is still to be optimized. The combination of an AC electric field with a small temperature gradient leads to a strong electrothermal flow that can be used for multiple purposes. Combining simulations and experiments, an analysis of the performance of electrothermal flow is provided when the temperature gradient is generated by illuminating plasmonic nanoparticles in suspension with a near-resonance laser.

Fluid flow is measured by tracking the velocity of fluorescent tracer microparticles in suspension as a function of the electric field, laser power, and concentration of plasmonic particles. Among other results, a non-linear relationship is found between the velocity of the fluid and particle concentration, which is justified in terms of multiple scattering-absorption events, involving aggregates of nanoparticles, that lead to enhanced absorption when the concentration is raised.

COMSOL Multiphysics simulations provide a description of the phenomenon that is compatible with experiments and constitute a way to understand and estimate the absorption and scattering cross-sections of both dispersed particles and/or aggregates. A comparison of experiments and simulations suggests that there is some aggregation of the gold nanoparticles by forming clusters of about 2-7 particles, but no

information about their structure can be obtained without further theoretical and experimental developments. This nonlinear behavior could be useful to get very high ETP velocities by inducing some controlled aggregation of the particles.

Fractal analysis of molecular microscopic dendritic aggregates: Beauty emerges from chaos

1st author

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Abstract

A myriad of complex disordered systems in nature exhibit dendritic patterns that can be described within the framework of fractal geometry. The latter has garnered much interest in comprehensively studying arrangements grown far from equilibrium, particularly in surface science. Neither crystalline nor completely amorphous, strongly disordered systems such as colloidal aggregates, polymers or dendritic crystals can't be understood employing classic concepts such as unit cells, Root mean square (RMS) or surface steps. Moreover, fractal nonintegral dimensions provide a new playground for exploring physical phenomena that cannot be quantified otherwise since they coincide or vanish in standard Euclidean space.

Organic molecules\' on-surface nucleation, growth, and aggregation can mainly be rationalised within fractal geometry. The existing scarce literature mainly reported molecular aggregates obtained in solution, and the few works that explored vacuum-deposited molecules only considered dilute systems with low coverage below the monolayer, where ramified snowflake-like or round islands with smooth edges that evolve into compact films were reported.

The present study aims to comprehensively elucidate the formation of unprecedented solid-state processed, long-range ordered and self-aggregated polar Boron subphthalocyanine chloride (BsubPc-Cl) chromophores. BsubPc-Cl is a well-known electron donor, which has been reported in several publications, where it is presented as a promising candidate for optoelectronic applications. Yet, to our knowledge, there is no mention in the literature of self-aggregation, which can seriously alter the device\'s performance. By investigating the morphology and photoluminescence dependence on the deposited film\'s nominal thickness and the aggregate\'s fractal properties, we delve into underlying phenomena and implications for organic electronic technologies.

Stochastic Precession Relaxation

1st author

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Abstract

Although the rigid body concept is of paramount importance in classical mechanics, one of its fundamental hypotheses, that the distance between any two constituent particles remains constant in time, fails in any real body due to elasticity and intrinsic thermal fluctuations. A model considering these effects has recently

been introduced in the literature [1]. This model predicts that a quasirigid body with zero angular momentum explores all orientations uniformly through thermal fluctuations. When the body spins, the equations describe an alignment process of the major principal axis with the angular momentum vector, resulting in increased temperature. This effect is known as precession relaxation. The theory also predicts the equilibrium shape of a spinning body. In the present work, we demonstrate that, in the absence of angular momentum, the theory predicts that principal axis unit vectors of a body undergo an anisotropic Brownian motion on the unit sphere, with the anisotropy arising from the different inertia moments of the body. We also show that the equilibrium time correlation function of the principal eigenvectors decay exponentially. This theoretical prediction is confirmed in molecular dynamics simulations of small bodies. The comparison of theory and equilibrium simulations allows us to measure the orientational diffusion tensor. We then use this information in the Stochastic Dissipative Euler's Equations, to describe a non-equilibrium situation of a body spinning around the unstable intermediate axis. The agreement between theory and simulations is excellent, offering a validation of the theoretical framework.

[1] P. Español, M. Thachuk, and J. De La Torre, European Journal of Mechanics - A/Solids 103, 105184 (2024), ISSN09977538

How complex is to be a hub? Dynamical complexity and the structure of complex networks

1st author

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Abstract

Since the beginning of the research on the dynamics of complex networks, the deep relationship between topology and dynamics has been thoroughly explored with regard to the synchronization between the nodes' dynamics, and the knowledge gathered so far has driven the advance in crucial applications. However, there are cases in which the system performs its activity in a partial or weak synchronization regime to preserve the balance between functional integration and segregation, whereas full synchronization is pathological. But even in a state far from synchronized, each coupled unit encodes the signature of its structural role in its own dynamics. We explore how this prominent feature could be used to extract information about the network without needing to reference pairwise correlations, even in situations where the structure is unknown. The coupling strength's effect against the nodes' dynamical complexity is found to be a function of their topological roles, with nodes of higher degrees displaying lower levels of complexity. Importantly, our results imply that it is possible to infer the degree distribution of a network only from individual dynamical measurements in a large variety of systems.

Portfolio optimization: from mathematical modeling to financial freedom

1st author

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Abstract

In this talk we will very briefly summarize the mathematical description of the financial problem of optimizing a portfolio in a Black-Scholes market in the presence of asymmetric information. Precisely, our portfolio will combine a riskless asset and a risky one, given by geometric Brownian motion. We will consider the case of two traders who possess different information on the market dynamics. The calculations will be carried out employing anticipative stochastic calculus and the emphasis of the talk will be put on one of our recent contributions to the subject. The focus will be on mathematical modeling rather than on the stochastic analytical details of the computations. In particular, we will discuss how the model assumptions are critical to derive conclusions that are financially meaningful. Moreover, we will frame this mathematical optimization problem in the actual financial practice within the regulatory system

of the European Union, which forbids insider information. With this we will try to illustrate how mathematical modeling can, in principle, go beyond scientific papers and become useful to protect the financial freedom of honest investors. All in all, we will try to convince the listeners how finance is a truly complex system that needs to be approached with interdisciplinary methods that include the mathematical and physical ones, among others; but more crucially we will try to be persuasive on how important it is to treat it this way for the potentially transcendent results that such an approach may give.

Using complex networks as efficient reservoirs in machine learning. An application to anticipating food price crises

1st author

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Co-authors

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Abstract

Anticipating price crises in the market of agri-commodities is critical to guarantee both the sustainability of the food system and to ensure food security. However, this is not an easy task, since the problem implies analyzing small and very volatile time series, which are highly influenced by external factors. In this communication we show that suitable reservoir computing algorithms can be developed that outperform traditional approaches, by reducing the Mean Absolute Error and, more importantly, increasing the Market Direction Accuracy. For this purpose, the applicability of five variants of such method to forecast this market is explored, and their performance evaluated by comparing the results with those obtained with the standard LSTM and SARIMA benchmarks. We conclude that decomposing the time series and modeling each component with a separate RC is essential to successfully anticipate price trends, and that this method works even in the complex changing temporal scenario of the Covid-19 pandemic, when part of the data were collected.

Cascading Failures in the US Banking Network - An Application of Complex Networks

1st author

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Abstract

We model the failure of a banking network due to the fall in asset prices by analyzing the top 100 banks holding 85% of the assets of the entire US banking system. The nodes are banking institutions, and the directed and weighted edges are the cross-holdings of shares between those banks, where for the first time, we have compiled the real cross-holdings between banks and the actual value of assets and liabilities from public data available.

To study the effect of the cross-holdings in the evolution of a bank's financial status, we follow its value (assets minus liabilities), and consider the effect of the loss of value of the prices of a fixed subset of their assets. When the value of any bank becomes negative, indicating its failure, we consider an extra factor reflecting the shock produced by the run on the bank, which results in further decrease of the values of its assets; through the effect of the cross-holdings, which can trigger the cascade of failures.

Due to the correlation between the size of the assets of banks and their out-degree (a small subset of them having the largest assets are also very diversified, possessing assets of many other banks) we considered the community structure of the network, using machine learning methods to identify the

clusters and also by looking at the standard Euclidean distance on a multi-dimensional space of centrality measures. As a consequence of this, we find that reducing the prices of assets substantially in one or two banks leads to the failure of many banks in the same cluster, but the impact of the cascade does not spread to other clusters

We will present strategies for applying possible cross-holdings constraint schemes to minimize the number of bank failures for a given price reduction level in assets.

Dynamics of the tragedy of the commons game

1st author

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Abstract

El concepto de uso excesivo de bienes comunes fue discutido por primera vez por W. Foster Lloyd en 1832 [1]. El influyente artículo de G. Hardin de 1968 [2] acuñó el término "tragedia de los bienes comunes", enfatizando metafóricamente cómo el libre acceso a recursos finitos conduce a la sobreexplotación.

Sobre la base de esta base, una extensa investigación ha analizado la gestión de bienes públicos, a menudo modelándola como un juego.

En este trabajo, exploramos la dinámica de la Tragedia del Juego de los Comunes desde una perspectiva de juego continuo, donde dos jugadores consumen un recurso común. Utilizando funciones de pago de tipo Cournot, limitamos la ingesta total de recursos a su capacidad máxima. El beneficio marginal unitario se vuelve cero si se excede el límite de recursos comunes (G_{max}) (tragedia). Introducimos un parámetro k para controlar la elasticidad del modelo y también analizamos el impacto del entrelazamiento cuántico entre jugadores (juego cuántico) [3].

El comportamiento de la dinámica se estudia considerando cómo varían los puntos fijos (particularmente el equilibrio de Nash) y la estabilidad del sistema en función de los diferentes valores de los parámetros involucrados en el modelo. Se estudia en qué casos el recurso puede estar sobreexplotado, ajustando los parámetros del modelo para evitar este escenario cuando sea posible. Los resultados se obtienen desde un punto de vista analítico y numérico utilizando diagramas de bifurcación para mostrar el comportamiento de la dinámica.

[1] Lloyd, WF Dos conferencias sobre los controles a la población. Popular. Desarrollo. Rev. 1833, 6, 473–496.

[2] Hardin, G. La tragedia de los comunes. *Ciencia* 1968, 162, 1243–1248.

[3] Grau-Climent, J.; García-Pérez, L.; Alonso-Sanz, R.; Losada, JC Dinámica de un juego cuántico de recursos comunes con expectativas de jugadores homogéneos. *Entropía* 2023, 25, 1585

Discovering dynamic laws from observations: the case of self-propelled, interacting colloids

1st author

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Abstract

Active matter spans a wide range of time and length scales, from groups of cells and synthetic self-propelled colloids to schools of fish and flocks of birds.

The theoretical framework describing these systems has shown tremendous success in finding universal phenomenology.

However, further progress is often burdened by the difficulty of determining the forces controlling the dynamics of individual elements within each system. Accessing this local information is pivotal for the understanding of the physics governing an ensemble of active particles and for the creation of numerical models capable of explaining the observed collective phenomena.

For this purpose, we have proposed a machine-learning tool, ActiveNet, that uses the collective movement of particles to learn one and two body forces acting on each particle. ActiveNet has been tested on simulations of Active Brownian particles (either repulsive or attractive), Active particles undergoing underdamped Langevin dynamics, and chiral active Brownian particles. We have demonstrated that ActiveNet can equally learn conservative or non-conservative forces as well as torques. Finally, we have applied ActiveNet to experiments of electrophoretic Janus particles, extracting the active and two-body forces that control the colloids' dynamics.

We believe that the proposed methodological tool, ActiveNet, might open a new avenue for the study and modeling of experimental suspensions of active particles.

Study of the epidemiological models based on differential equations. An application to COVID-19 in Beniel (Murcia)

1st author

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Abstract

From the plague and smallpox centuries ago to the recent COVID-19 pandemic, human beings have been dealing with diseases during our whole existence. Epidemiology uses deterministic as well as stochastic models to understand the spread of the diseases in the past and to predict the impact of the incoming ones [1]. These models consider that each individual belongs to a compartment, and each group relates to the others by rates. Examples of these models are the SIR model, the SEIR model, the SIS model, the SIRS model or the SEIS model [2]. In this work we apply the SEIR model to analyze the evolution of the third wave of the pandemic of COVID-19 in Beniel (Murcia), considering two scenarios. In the first one, the contagion rate β is assumed to be constant, while in the second one it varies with time, $\beta(t)$, according to the model proposed by Gutiérrez and Varona [3], which considers the preventive measures adopted at any given time by the governors as well as the behaviour of the population in the face of the pandemic. The results obtained in our study show a nice agreement with government data [4].

[1] I. Sanz Garayalde, Modelos epidemiológicos basados en ecuaciones diferenciales. Trabajo Fin de Grado, Universidad de La Rioja (2015-2016).

[2] J. Duoandikoetxea, El modelo SIR, un enfoque matemático de la propagación de infecciones. <https://culturacientifica.com/2020/08/24/el-modelo-sir-un-enfoque-matematico-de-la-propagacion-de-infecciones/> (2020).

[3] J. M. Gutiérrez, J. L. Varona, Análisis de la posible evolución de la epidemia de coronavirus COVID-19 mediante un modelo SEIR. Informe, Universidad de La Rioja (2020).

[4] Servicio de Epidemiología. Región de Murcia. Histórico de informes epidemiológicos. <https://www.murciasalud.es/web/servicio-de-epidemiologia/historico-informes-epidemiologicos>. Último acceso: 18 de marzo de 2024.

Non-locality and Casimir effects on 3D short-ranged critical wetting: a renormalization-group study.

1st author

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Abstract

In this contribution we will analyze the effect that non-locality and the Casimir-like contribution to the binding potential have on the critical wetting for short-ranged forces. As capillary waves are still the relevant fluctuations for 3D short-ranged critical wetting, we will extend previous linear and non-linear functional renormalization-group approaches to our case. We will compare our results with previous Ising model simulations, finding that they agree with the preasymptotic regime we observe in our RG calculations in the same range of system sizes. This may explain the discrepancies in the critical exponents observed between Ising simulation results and the RG predictions.

(Optimal) Control Theory in Stochastic Processes

1st author

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Abstract

The concept of control goes beyond natural and mathematical sciences. It is a human ambition that persists from the origin of our species. In fact, control is sought in production of artworks, healthy human behavior, and an endless number of daily examples. The modern mathematical formulation of optimal control theory (OCT) dates back to the 50's of the 20th century and its development is associated with the Space Race and optimal design of aircrafts. This is why optimal control has been typically considered as an "engineering" tool and its application to fundamental problems in physics has been really scarce. How can a statistical physicist contribute to this long-term human project?

In the last decades, we have witnessed a new rise of endeavors to take advantage of control theory in fundamental physics. On the one hand, the so-called shortcuts to adiabaticity in quantum mechanics were introduced as successful protocols to manipulate and prepare quantum states. Herein, adiabaticity means quasistatic and has nothing to do with the thermodynamic heat. On the other hand, more recently, the same kind of strategies has been brought into the context of statistical mechanics and stochastic processes. Since adiabaticity is not always a desirable reference, the general term swift state-to-state transformations (SST) was coined to embrace the entire catalogue of possible shortcutting.

This contribution intends to give an overview of these appealing techniques, showing the versatility and power of control theory to solve physically interesting problems. For the sake of concreteness, we take an overdamped Brownian particle in the presence of a trapping potential as our model system. Even with this simple but general setup, we will be able to illustrate different shortcutting strategies and different

optimization procedures depending on the figure of merit: maximum work extraction, minimum connection time, etc.

Feedback-controlled systems: Markovian description and refinements of the second law

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Abstract

The role played by information in the thermodynamic balance of feedback-controlled systems has been shown to be crucial, when computing several physical quantities such as the entropy or the efficiency of the system. This is the case of the feedback flashing ratchet, where an overdamped Brownian particle is submitted to a periodic potential that is modified by the action of an external controller. This feedback controller measures the particles position at periodic times and modifies the state of the potential, depending on the outcome of the measurement.

A Markovian description of a general class of feedback-controlled systems—which include as a particular case the feedback flashing ratchet—can be built, by considering the joint process defined by the instantaneous position of the particle and the control state (X,C) : the corresponding probability density $P(x,c,t)$ obeys a differential Chapman-Kolmogorov differential equation. In addition, an H-theorem is proved, which ensures the convergence of $P(x,c,t)$ to a periodic long-time state, independent of the initial conditions.

Within the Markovian picture, a thermodynamic balance is developed to identify the work performed by the particle, the heat exchanged with the bath, and the entropy of the joint process. It is especially insightful to link the entropy in the Markovian picture with the one derived when considering the full history of the controller, since this connection may clarify the role played by information in the system. In addition, refinements of the second law of thermodynamics are achieved by splitting the entropy production into different contributions, analogous to the Hatano-Sasa decomposition. These refinements of the second law may entail tighter bounds for the entropy production in the long-time state.

Entropy-based early detection of critical transitions in spatial vegetation fields

1st author

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Co-author

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Abstract

In semiarid regions, vegetated ecosystems can display abrupt and unexpected changes, i.e., transitions to different states, due to drifting or time-varying parameters, with severe consequences for the ecosystem and the communities depending on it. Despite intensive research, the early identification of an approaching critical point from observations is still an open challenge. Many data analysis techniques have been proposed, but their performance depends on the system and on the characteristics of the observed data (the resolution, the level of noise, the existence of unobserved variables, etc.). Here, we propose an entropy-based approach to identify an upcoming transition in spatiotemporal data. We apply this approach to observational vegetation data and simulations from two models of vegetation dynamics to infer the

arrival of an abrupt shift to an arid state. We show that the permutation entropy (PE) computed from the probabilities of two-dimensional ordinal patterns may provide an early warning indicator of an approaching tipping point, as it may display a maximum (or minimum) before decreasing (or increasing) as the transition approaches. Like other spatial early warning indicators, the spatial permutation entropy does not need a time series of the system dynamics, and it is suited for spatially extended systems evolving on long time scales, like vegetation plots. We quantify its performance and show that, depending on the system and data, the performance can be better, similar or worse than the spatial correlation. Hence, we propose the spatial PE as an additional indicator to try to anticipate regime shifts in vegetated ecosystems.

POSTER: Shaping coral reef growth. The role of nutrient diffusion and erosion.

Presenter

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Co-presenter

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Abstract

Coral reefs are some of the most biodiverse and productive ecosystems in the world, providing habitats for a vast array of marine species and supporting the livelihoods of millions of people. However, coral reefs are facing increasing threats from climate change, pollution and overfishing. Understanding how these ecosystems grow and function is crucial for effective conservation efforts. One key aspect of coral reef ecosystems is their spatial patterns, which can provide important insights into how these ecosystems form and persist. Remote sensing data and satellite imagery have revealed that coral reefs often exhibit distinct patterns in their morphology, such as the arrangement of coral colonies and the formation of reef structures. These patterns can reflect a combination of biological and physical processes, including water flow, nutrient availability, and competition among coral colonies and reefs.

To better understand the mechanisms underlying coral reef pattern formation, a range of theoretical and numerical models based on reaction diffusion equations have been used to explore the roles of competition, predation, and other ecological factors in shaping coral reef communities. Other models have focused on the physical processes that influence reef growth, such as hydrodynamics and sediment transport. However, many of these models have limitations in terms of their ability to capture the complexity of coral reef ecosystems. While some of them overlook the importance of specific ecological interactions or physical processes, others are overly simplified, ignoring the heterogeneity of coral reef habitats or assuming uniform conditions across the reef.

We will propose a novel model that aims to address some of actual limitations by incorporating both biological and physical factors into a single framework. Specifically, we will focus on the role of nutrient diffusion and erosion in shaping the spatial patterns of coral reefs.

POSTER: Phase-space structures and vibrational motion in KCN molecular system

Presenter

Fabio Revuelta Peña Universidad Politécnica de Madrid

Co-presenters

Francisco Javier Arranz Universidad Politécnica de Madrid

Rosa María Benito Universidad Politécnica de Madrid

Florentino Borondo Universidad Autónoma de Madrid

Abstract

In this work, we analyze the evolution of the phase-space structures of KCN molecular system as a function of the vibrational energy using Lagrangian descriptors. For low energies, the motion is mostly regular around the absolute minimum of the potential energy surface. As the energy increases, the phase space combines regions with regular and chaotic motion, a difference that is well captured by the Lagrangian descriptors. Furthermore, we show a perfect agreement between the bifurcation theory and the differences in the phase-space structures shown by Lagrangian descriptors as the vibrational energy is modified.

POSTER: Mining data from social networks to explain social dynamics and polarization

Presenter

Alberto Perez Muñuzuri Universidade de Santiago de Compostela

Co-presenters

Santiago Paramés-Estévez Universidade de Santiago de Compostela

Alejandro Carballosa Universidade de Santiago de Compostela

David Garcia-Selfa CESGA (Supercomputing Center of Galicia)

Abstract

Social networks are the paradigm for our society; everything that happens is reflected in them and they strongly influence our social dynamics. Thus, it becomes crucial to understand the way they are organized in order to fully understand the social processes taken place nowadays. We exemplify the problem by extracting data freely available in a commonly used social network, Twitter, building up a complex network that describes the online activity patterns of society. These networks are composed of a huge number of nodes and an even larger number of connections, making it extremely difficult to extract meaningful data that summarizes and/or describes behaviors. We propose techniques to extract data from these networks and analyze it to extract relevant information. In the first part of the contribution, we use artificial intelligence tools to analyze the system and obtain the topological parameters describing the networks. In the second part of the contribution, we focus on a phenomenon that is characteristic of many of the western societies; polarization or the tendency to develop two opposed opinions in almost any topic. Using nonlinear dynamic techniques we propose that the topological structure of the network provides hints of how likely it is to become polarized.

Santiago Paramés-Estévez, Alejandro Carballosa, David Garcia-Selfa and Alberto P. Munuzuri. Artificial intelligence techniques used to extract relevant information from complex social networks. *Entropy* 25(3), 507 (2023)

Alejandro Carballosa, Álvaro Crego and Alberto P. Muñuzuri. Quantifying the potentiality for polarization in opinion networks. *Chaos, Solitons and Fractals* 173, 113697 (2023)

POSTER: Task-driven flexibility is mediated by integration, not segregation, of brain networks

Presenter

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Abstract

Our study approaches the brain as a complex system, employing statistical physics lens to scrutinize its macro-scale modular organization and adaptive mechanisms during various cognitive tasks. Through a multimodal analysis, we explored both the structural and functional networks of the brain. Structural connectivity is characterized by white matter pathways, whereas functional connectivity arises from the statistical correlations in neuronal activity. We introduced two primary metrics within a shared latent space—modular structure-function coupling and modular functional connectivity—and calculated the ratios between these metrics during task performance and resting states. These metrics were examined both intra-modularly, to detect modular segregation, and inter-modularly, to assess modular integration. Our findings demonstrate that the brain's task-driven flexibility is primarily facilitated by network integration, underscoring the brain's ability to reconfigure itself efficiently rather than relying on segregation. This study highlights the crucial role of computational and statistical methods in decoding the complex dynamics of neural functionality.

POSTER: Permutation entropy-based characterization of speckle patterns generated by semiconductor laser light

Presenter

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Abstract

Semiconductor lasers with optical feedback are stochastic nonlinear systems that can display complex dynamics and abrupt changes when their operation conditions change. Even very small changes can lead to large variations in the spatial and spectral properties of the laser emission. This makes a semiconductor laser with feedback an ideal system for conducting controlled experiments to test data analysis tools to detect and characterize transitions. Here, we identify feedback-induced transitions by analyzing speckle patterns that are generated after the laser light propagates in an optical fiber. Speckle patterns result from the interference of multiple modes, and their statistical properties are understood, but a direct mathematical model does not exist. Here we show the versatility of the correlation length and the permutation entropy as measures for characterizing speckle patterns. Combining entropy and correlation analysis with speckle contrast analysis, we uncover changes that occur when the laser current increases from below to well above the threshold, which unveils the effects of optical feedback on the coherence of the laser emission.

POSTER: Numerical methods for stochastic simulations: application to contagion processes

Presenter

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Abstract

Stochastic modeling has become one of the main pillars of complexity science. As models become more intricate, there arises a technical challenge of producing numerically stochastic trajectories in feasible computation times, since unbiased methods, those that generate statistically unbiased realizations of stochastic trajectories, like the Gillespie algorithm, may become unpractical due to lengthy computations. In this work, we analyze the issue on whether the binomial method is competitive compared to unbiased methods. We provide numerical and analytical evidence that the systematic errors of the binomial method scale linearly with the discretization time. Using this result, we establish a rule for selecting the optimal discretization time and number of simulations required to estimate averages with a fixed precision while minimizing CPU time consumption and derive a rule of simple and practical use that tells us in which cases the binomial method is superior to unbiased algorithms. We quantify the relative efficiency of the binomial versus the unbiased method as the ratio of CPU times taken by each method to achieve a desired precision. The advantage of using the binomial method depends on the target precision: unbiased methods become more optimal as the target precision increases or as the number of agents increases. In summary, this work provides a solution for the existing debate regarding the use of the binomial approximation to sample stochastic trajectories. The discretization time of the binomial method needs to be chosen carefully since large values can result in errors beyond the desired precision, while low values can produce extremely inefficient simulations. A proper balance between precision and CPU time consumption is necessary to fully exploit the potential of this approximation and make it useful. The efficiency of the binomial method is superior to the unbiased approaches only when the target precision is above a certain threshold value.

POSTER: Unveiling the social forces that drive polarization in multipolar social systems

Presenter

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Abstract

Social polarization is a growing concern worldwide, as it strains social relations, erodes trust in institutions, and thus hurts democratic societies. Polarization has been traditionally studied in binary conflicts where two groups support opposite ideas. However, in many social systems, such as multi-party democracies, political conflicts involve multiple dissenting factions. Despite the prevalence of multipolar systems, there is still a lack of suitable analytical tools to study their polarization patterns. In this work, we introduce new polarization metrics for multidimensional scenarios and develop a methodology that extracts the ideological structure of multipolar contexts from social networks. We propose the trace of the covariance matrix (the total variation) of the multipolar opinion distribution as a measure of global polarization, and its eigendecomposition to identify the directions of maximum polarization. Instead of using a pre-conceived opinion space (conservative vs progressive, liberal vs authoritarian, etc.), our framework reveals the natural ideological axes of the system. We apply our methodology to quadripolar and pentapolar real-world democratic processes, finding non-trivial ideological structures with clear connections to the underlying social context. Our framework opens new avenues for understanding multilateral social tensions and facing the challenges of polarization in a unified way [1].

[1] Samuel Martin-Gutierrez, Juan C. Losada, Rosa M. Benito, Multipolar social systems: Measuring polarization beyond dichotomous contexts, *Chaos, Solitons & Fractals*, 169, 113244 (2023). <https://doi.org/10.1016/j.chaos.2023.113244>

POSTER: Random walks in granular systems

Presenter

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Abstract

We investigate the diffusive behaviour of a tagged spherical particle (intruder) in granular systems constituted by smooth hard spheres (grains). We consider a freely cooling dry granular gas (system 1) [1] and a granular suspension in which both intruder and granular gas are immersed in an interstitial fluid (system 2) [2]. In this latter case, we adopt a coarse-grained approach where the effect of the interstitial fluid on grains is accounted for via an effective fluid-solid force [3]. Both the intruder-grain collisions and the grain-grain collisions are, in general, inelastic. In system 2, the interstitial fluid plays the role of a thermal bath which has a two-fold effect: on the one hand, it feeds both intruder and grains with energy; on the other hand, it exerts a viscous drag on them. This thermal bath acts as a thermostat which drives the gas into a non-equilibrium steady state. In such a state, the respective granular temperatures of both intruder and grains (i.e., their mean kinetic energies) take constant values. With the help of a Chapman-Enskog approach, we compute for both systems explicit expressions of the intruder's mean square displacement (MSD). In system 1, the MSD exhibits a logarithmic time dependence (ultraslow diffusion), as opposed to the linear time dependence observed for system 2 (normal diffusion). In both cases, we find regimes with a non-monotonic dependence of the MSD on the normal restitution coefficient for grain-grain collisions. These results are confirmed by DSMC simulations and intuitively interpreted in terms of an effective random walk picture.

[1] E. Abad, S.B. Yuste, and V. Garzó, *Granular Matter* 24, 1-19 (2022).

[2] R. Gómez González, E. Abad, S.B. Yuste, and V. Garzó, *Phys. Rev. E* 108, 024903 (2023).

[3] V. Garzó, S. Tenneti, S. Subramaniam, and C. M. Hrenya, *J. Fluid Mech.* 712, 129-168 (2012).

POSTER: Dynamics of a confined and ultraconfined system

Presenter

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Abstract

This work will be focused on studying the dynamics of a system composed of inelastic hard spheres or disks that are confined between two parallel vertically vibrating walls (the vertical direction is defined as the direction perpendicular to the walls). The distance between the two walls is supposed to be larger than twice the diameter of the particles so that the particles can pass over each other, but is still much smaller than the dimensions of the walls. Hence, the system can be considered to be quasi-two-dimensional (quasi-one-dimensional). For dilute systems, a closed evolution equation for the one-particle distribution function is formulated that takes into account the effects of the confinement. The kinetic equation is solved approximating the distribution function by a two-temperature (horizontal and vertical) Gaussian distribution. The obtained evolution equations for the partial temperatures are solved, finding a very good

agreement with molecular dynamics simulation results for a wide range of parameters (inelasticity, height and density) for states whose projection over a plane parallel to the walls is homogeneous. The effective equation of state in the plane is analyzed and related with the presence of an instability in which the homogeneous state is unstable. Finally, the case of elastic particles confined between reflecting parallel walls is considered. The diffusion in the plane is studied finding normal diffusion with explicit values of the effective diffusion coefficient. A good agreement with molecular dynamics simulations is found.

POSTER: Optimal investment with insider information using Skorokhod & Russo-Vallois stochastic integration

Presenter

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Co-presenters

Carlos Escudero Universidad Nacional de Educación a Distancia

Tomoyuki Ichiba University of California, Santa Barbara

Abstract

We are interested in portfolio optimization using insider information with different stochastic noise interpretations of the insider wealth dynamics, where we allow the portfolio to anticipate future information. We model the noise with two types of stochastic integrals: the Russo-Vallois forward integral and the Skorokhod integral. Both generalize the Itô integral. We conclude that although the forward integral leads to more expected wealth in a single-period setting, in a continuous setting, using the Skorokhod integral is more profitable. Therefore, it better models an insider in this context.

POSTER: Optimal heterogeneous resetting for Brownian searchers

Presenter

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Co-presenters

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Abstract

Stochastic resetting was introduced as a mechanism to improve Brownian search strategies. At certain random times, the searcher restarts its natural dynamics, forgetting the past and beginning to search again until it reaches the target. For the simplest case of one-dimensional searcher, Poissonian stochastic resetting renders the average time to hit a fixed target, also known as the mean-first passage time (MFPT), finite. The ability of making the MFPT finite is an appealing property that has arisen the interest of the statistical physics community, since an optimisation problem appears searching the optimal rate that minimises the MFPT. Furthermore, broadly speaking, search processes with stochastic resetting have many applications in a wide range of contexts beyond theoretical physics, such as animal foraging, site-binding search of biomolecules in chemical reactions. Previous works about stochastic resetting usually considers a single fixed target that remains at the same position. Nevertheless, from a fundamental point of view, the searcher does not know where its objective is, i.e. there is some degree of randomness in the search process that renders every instance thereof unique. It is then natural to wonder how the information about the target position distribution (disorder) can guide a searcher. In this work, we address search processes with quenched (or static) disorder, i.e. the position of the target follows a certain static

spatial distribution. This raises two questions. 1) How does disorder affect the search process? 2) Is it possible to define clever strategies for a global optimisation of MFPT, e.g. an optimal space-dependent reset given the target position distribution? These questions define an challenging optimal control problem with interesting applications within the context of Brownian searchers.

POSTER: Optimal synchronisation to a limit cycle: the Van der Pol oscillator

Presenter

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Co-presenters

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Antonio Prados Montaña Universidad de Sevilla

Abstract

In the absence of external forcing, in the Van der Pol oscillator, all trajectories in phase space tend to a closed, periodic trajectory—the limit cycle—after infinite time. Our main goal is to reach this limit cycle in a finite time by applying a tailored external force protocol that minimises the work done by this force, i.e. the energetic cost of the protocol. When the applied force has no bounds, the minimisation of the work can be solved by applying calculus of variations, which leads to a Euler-Lagrange equation for the optimal trajectory. When the applied force is bounded, this non-holonomic constraint makes it necessary to resort to optimal control theory tools. Maximum Pontryagin's Principle tells us that the optimal trajectory comprises several stages, which alternate between bang and Euler-Lagrange pieces. Also, we consider the brachistochrone problem, i.e. minimising the time needed to reach the limit cycle. Finally, we briefly study the relation between both optimal control problems.

Nuclear Physics Specialized Group Symposium / Grupo Especializado de Física Nuclear (GEFN)

Organiser

Dolores Cortina, IFIC Alejandro Algorta (IFIC) Carlos Guerrero (US) Laura Tolos (ICE) Tomás R. Rodríguez (UCM)

Abstract

The RSEF specialized group symposium on Nuclear Physics, which will take place at the XXXIX Biennial Meeting, aims to be a forum to relate researchers in this field and communicate advances in Nuclear Physics in its different lines of research, among others: theory, modelling, AI and ML, experiments, facilities, detectors, data analysis and applications.

El simposio de grupo especializado en Física Nuclear de la RSEF, que va a desarrollarse en la XXXIX Reunión Bienal tiene como objetivo ser un foro para relacionar a los investigadores en este campo y comunicar los avances en Física Nuclear en sus distintas líneas de investigación, entre otras: teoría, modelado, AI y ML, experimentos, instalaciones, detectores, análisis de datos, y aplicaciones.

List of abstracts at the symposium

Advancing Neutron Safety and Dosimetry in Nuclear Facilities: The Development and Application of NEREIDA

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Abstract

The development of nuclear facilities, particularly those generating fast neutrons like the CLPU or the forthcoming IFMIF-DONES, demands reliable tools for designing, licensing and safety assessments. NEREIDA (NEutrones Rápidos para la Explotación de Instalaciones con Dispositivos Atómicos) emerges as an innovative and autonomous tool designed to meet this need. Utilising Monte Carlo methods based on Geant4, NEREIDA offers the capability to accurately characterise the three-dimensional neutron flux spectrum, from the thermal to the high-energy component within such installations, and to calculate key dosimetric magnitudes of interest, including ambient and personal dose equivalents, $H^*(10)$ and $H_p(10)$, respectively. This tool incorporates state-of-the-art algorithms and libraries for neutron transport, interaction, moderation, and material neutron activation, aligning with the latest standards. Its user-friendly interface will facilitate the generation of the Geant4-based model of the facility from CAD files, material data, and neutron source characteristics of any kind, requiring no programming expertise. The data generated by NEREIDA will adhere to the FAIR principles, ensuring it is Findable, Accessible, Interoperable, and Reusable, thereby facilitating broader scientific collaboration in the field. An additional feature of NEREIDA is its enhanced simulation of cosmic ray background radiation effects, considering realistic atmospheric and geomagnetic conditions, and the moderation of cosmic neutrons. Moreover, it includes two gender-based anthropomorphic phantoms to assess the expected effective dose, significantly improving safety assessments for inadvertent human exposure during irradiation sessions. Validation of

NEREIDA is being conducted through comparison with experimental simulations and measurements, focusing on signals in a different type of neutron detectors and the spatial neutron spectrum distribution at the Laboratorio de Patrones Neutrónicos (LPN, CIEMAT, Spain). This work will detail NEREIDA's status, validation outcomes, and future developments, showcasing its potential to contribute to the characterisation of neutron phenomena in nuclear facilities and the enhancement of safety protocols.

Spectrometry of cosmic-ray neutrons with HENSA++: commissioning and project status

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Abstract

Neutrons are produced continuously as a secondary radiation from cosmic-rays interactions in the upper atmosphere of our planet. The characterization of such secondary neutrons is connected with different fields such as environmental radioactivity [1] and the physics of cosmic-rays and space weather [2].

The High Efficiency Neutron Spectrometry Array (HENSA) is a collaboration focused on the design and development of high efficiency neutron spectrometers [3]. The latest version of this project, HENSA++, is intended for high efficiency measurements of cosmic-ray neutrons, focusing on space weather and environmental dosimetry applications. The operation of HENSA++ is based on the same principle that the Bonner Spheres Spectrometers (BSS) [4]. A topological modification of the detector geometry has enabled to improve the detection efficiency between 5 up to 10 times over the standard BSS [4]. The current version of HENSA++ is composed by an array of sixteen He-3 tubes, each one embedded in different materials including high density polyethylene moderators, cadmium shieldings and lead neutron converters. This setup allows for spectral sensitivity from thermal up to GeV's neutrons and provides near real-time measurements of the neutron spectrum on a time scale of tens of minutes up to few hours, thus enabling possible applications in space weather as a neutron monitor with spectral sensitivity.

In the present work, the details about the design and optimization of HENSA++ and the commissioning of the spectrometer for cosmic-ray neutron measurements are presented. Additionally, the challenges for the reconstruction of wide energy range spectra (thermal up to 1 GeV) from BSS measurements are discussed.

[1] European Radiation Dosimetry Group (2004). Report 140: Cosmic Radiation Exposure of Aircraft Crew.

[2] J. A. Simpson (2000). Space Science Reviews, 93, p. 11–32.

[3] <https://www.hensaproject.org/>

[4] D.J. Thomas and A.V. Alevra (2002). NIMA, 476, p. 12–20.

High precision $^{209}\text{Bi}(n,?)$ cross section measurement at n_TOF EAR2.

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Abstract

Innovative of future nuclear reactor designs and safety during operation relies on the accuracy of nuclear data, and in particular on the minimization of the uncertainty in microscopic nuclear cross sections. MYRRHA is an experimental Accelerator Driven System cooled by a lead-bismuth mixture. The radiological burden associated with the use of this type of coolant for fast nuclear systems is given by the production of ^{210}Po isotope from (n, γ) reactions on ^{209}Bi . There are significant discrepancies between different $^{209}\text{Bi}(n, \gamma)$ evaluations and the feeding to the metastable state, so only the accurate knowledge of both reaction channels and its branching ratio can accurately predict the inventory of ^{210}Po for lead-bismuth heavy coolant nuclear systems. From the astrophysical point of view, $^{209}\text{Bi}(n, \gamma)$ plays an important role in the of the s-process and for U/Th cosmic clocks.

The most recent $^{209}\text{Bi}(n, \gamma)$ ToF measurement was performed at CERN n_TOF EAR1 by C. Domingo and collaborators in 2006 using the state-of-the-art low neutron sensitivity C6D6 detectors. However the target uncertainty could not be reached due to a significant in-beam γ -ray background and insufficient EAR1 luminosity. This limitation has been significantly improved with the high luminosity EAR2 and refined spallation source design. Recently, in combination with the high sensitivity STED array detection setup, EAR2 has demonstrated its potential for challenging (n, γ) cross section measurements in a broad neutron energy range.

The goals of the present $^{209}\text{Bi}(n, \gamma)$ experiment is to get a 5-10% accuracy in Resolved Resonance Region covering neutron energies range from thermal up to 35 keV and less than 15% accuracy in the neutron energy range from 35-100 keV. At the time of the conference we will present a comprehensive and full view of the experiment currently carried out at the CERN n_TOF facility and the first experimental results from the ongoing campaign.

First results of the neutron capture cross-section measurement of $^{146}\text{Nd}(n, \gamma)$ @ n_TOF-EAR2

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Abstract

The study of the slow neutron capture process is fundamental for understanding the creation of isotopes heavier than ^{56}Fe in stars, as well as isotopic ratios.

The most precise observational data available on isotopic ratios produced by s-process nucleosynthesis is based on measurements of stardust silicon carbide (SiC) grains.

These measurements are in disagreement with recent model predictions for the Nd isotopes, [1,2,3], consistently predicting a 15% higher neutron-capture cross section of ^{146}Nd .

Furthermore, the current reference data for $^{146}\text{Nd}(n,?)$, by Bao et al. [4], is based on a measurement of the unresolved resonance region (URR), between 3 and 225 keV, by Wisshak [5], and shows discrepancies with other measurements.

With the aim of solving the discrepancies, an experimental campaign on the measurement of $^{146}\text{Nd}(n,?)$ at EAR2-n_TOF, [6], using a high sensitivity setup, [7], and a high-purity sample of ^{146}Nd has been approved to take place in the first half of 2024, [8].

This contribution will present a summary of the preliminary results of this campaign, covering the resolved resonance region (RRR) of ^{146}Nd up to 5 keV.

An outlook into a complementary campaign on the activation of $^{146}\text{Nd}(n,?)$ in a quasi-stellar spectra, yielding ^{147}Nd with a suitable half-life ($\sim 11\text{d}$) to directly determine the MACS, will be included.

- (1) S. Richter et al., Abstracts Lunar and Planetary Science Conf., 23, 1147, (1992)
- (2) T. R. Ireland et al., Geochimica et Cosmochimica Acta 221, 200-218 (2018)
- (3) Q.Z. Yin et al., The Astrophysical Journal, 647, 676–684 (2006)
- (4) Z.Y. Bao et al., Atomic Data Nucl. Data Tables 76, 70 (2000)
- (5) K. Wisshak et al., Phys. Rev. C 57, 391 (1998)
- (6) C. Weiss, Nucl. Inst. Methods A, 799, 90-98 (2015)
- (7) J. Lerendegui-Marco et al., EPJ Web Conf. 284, 01028 (2023)
- (8) J. Lerendegui-Marco et al., CERN-INTC-2023-055, INTC-P-671 (2024)

First full beta-strength measurement with DTAS across $N=126$ at FAIR PHASE-0

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(On behalf of [S505-DESPEC experiment collaboration](#))

Abstract

Our understanding of the production of the heavy elements in the Universe is still incomplete. In particular the contribution of the rapid neutron capture (r -) process to the observed stellar abundances around mass number $A \sim 195$ (the 3rd r -process peak), which is linked to the effect of $N=126$ shell closure in the production path. Given the lack of nuclear data, astrophysical abundance calculations must rely on theoretical predictions, for the important parameters $T_{1/2}$ (half-life) and P_n (neutron emission probability). Both parameters are extracted from theoretical beta-strength distributions, which depend on nuclear structure. However, large discrepancies exist among different theoretical models. Our aim is to discern between models by comparing with measured beta-strengths. For this we will use Total Absorption Gamma-ray Spectroscopy (TAGS) which is the most effective method for obtaining beta-strength distributions across the entire decay energy window.

With this purpose, an experiment was performed at the GSI/FAIR facility in June 2022. During the experiment, the decay of Hg, Au and Pt isotopes with $N=125-27$ were measured. These isotopes were produced by high-energy nuclear reactions using a beam of Pb on a Be target and selected and identified using the FFragment Separator (FRS). Ion implantations and decays particles were measured with the Advanced Implantation and Decay Array (AIDA), while isomeric and beta-delayed gamma-ray cascades were measured with the Decay Total Absorption Spectrometer (DTAS), both developed within the NUSTAR/DESPEC collaboration.

The manifold analysis of the data (FRS-AIDA-DTAS) is progressing. We succeeded in performing a preliminary ion identification and obtaining the first TAGS decay spectra by combining the information from the three systems. We will discuss the status of the analysis and the work remaining.

Study of actinide sources in the Baltic Sea by Accelerator Mass Spectrometry

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Abstract

The Baltic Sea has increased accumulation of radioactive materials compared to open oceans due to the impact of multiple regional sources: i) fallout from Chernobyl accident (1986), ii) liquid releases from Sellafield and La Hague nuclear reprocessing facilities transported through the North Sea, iii) authorized radioactive discharges from nuclear installations, and iv) possible leakages from the radioactive wastes dumping sites [1]. Moreover, all these regional inputs coexist with the baseline radioactivity levels imposed by the global fallout (GF) from the atmospheric nuclear tests (1945-1980) [2]. Although the Baltic Sea has been one of the most studied areas regarding radioactive radionuclides, long-lived actinides such as ^{236}U , ^{237}Np or Pu isotopes, have been scarcely investigated and there are still many open questions about their sources in this area. Accelerator Mass Spectrometry (AMS) has demonstrated its capability for the study of such family of radionuclides in environmental samples [3].

In this context, this work is focused on the study of the Tvären Bay, directly impacted by the liquid releases from Studsvik Nuclear facility (east coast of Sweden), whose actinide isotopic composition has not been documented. Using the 1 MV AMS system at the CNA (Centro Nacional de Aceleradores, Sevilla), the Pu isotopic distribution was studied in an undisturbed sediment core, including the most minor isotopes (^{241}Pu , ^{242}Pu , ^{244}Pu). Those results have allowed us to reconstruct Studsvik release history for plutonium [4]. This work is now being expanded to other radionuclides (^{233}U , ^{236}U , ^{237}Np) and the developed techniques will be finally applied for a complete study of the Baltic seabed.

[1] HELCOM (2018) Baltic Sea Environment Proceedings N151

[2] Hardy EP et al (1973) Nature 241:444–445

[3] Fifield LK (2008) Quat Geochronol 3:276–290

[4] López-Lora M et al (2023) Environ Sci Technol

Core destruction effects in nucleon removal reactions

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Abstract

Nucleon removal reactions at intermediate energies have proven to be a powerful tool to extract spectroscopic information from atomic nuclei. As these reactions explore similar nuclear properties it is

expected that different reaction yield consistent results. However, discrepancies have been found between the systematics for different nucleon-removal reactions. In particular, for intermediate-energy nucleon-knockout reactions with ^9Be and ^{12}C targets, a trend was found where cross sections were severely overestimated when removing the deficient species in asymmetric nuclei, but their magnitude was well-predicted for the more abundant species [1]. While originally this was thought to be related to short-range correlations in the nucleus, the fact that this trend has not been observed in transfer or knockout reactions with proton targets, i.e. (p,pN), points to some deficiencies in the description of the reactions [2]. In this work we study an effect that has been commonly ignored in usual reaction formalisms: the final-state interaction between the removed nucleon and the residual nucleus (core), which can lead to the excitation and destruction of the core, reducing the nucleon removal cross sections, which require core survival. This effect would be more intense when removing more deeply-bound nucleons, which interact more strongly with the core and thus seems a possible explanation for the isospin dependence of the overestimation for nucleon knockout reactions. We first study this effect in elastic breakup reactions, where both nucleon and core survive, by extending the state-of-the-art Continuum- Discretized Coupled-Channels (CDCC) formalism to include the interaction between nucleon and core via use of a complex potential, which requires the use of a biorthogonal basis [3]. We later present results to nucleon knockout reactions, where we use an effective nucleon density to account for the nucleon-core interaction, finding a reduction in the isospin-asymmetry dependence of the discrepancies between theory and experiment for selected cases [4].

[1] A. Gade et al, Phys. Rev. C 77, 044306 (2008)

[2] T. Aumann et al, Prog. Part. Nucl. Phys. 118, 103847 (2021)

[3] M. Gómez-Ramos, J. Gómez-Camacho and A.M. Moro, Phys. Lett. B 832, 137252 (2022)

[4] M. Gómez-Ramos, J. Gómez-Camacho and A.M. Moro, Phys. Lett. B 847, 138284 (2023)

The first miniTrasgo Cosmic Ray detector

1st author

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Abstract

(C. Soneira on behalf of the CASTRO collaboration). The study of cosmic rays, originating from various cosmic sources, presents ongoing challenges due to their high energies and elusive nature. The first miniTRASGO cosmic ray telescope, developed as part of the TRASGO project within the CASTRO collaboration is presented. The miniTRASGO employs Resistive Plate Chambers (RPCs) to detect ionizing secondary cosmic rays, namely muons, offering a cost-effective and versatile solution for cosmic ray detection. The system architecture and calibration procedures are outlined, along with results from measurements and analyses. Notably, the miniTRASGO demonstrates high efficiency and resolution in detecting cosmic ray events, providing valuable data for further studies. As a testament to its effectiveness, the miniTRASGO successfully identified a Forbush decrease event, showcasing its capability in monitoring cosmic ray fluctuations. Future work includes enhancements in particle identification, environmental optimization, and collaboration consolidation within the cosmic ray research community. Overall, the miniTRASGO telescope represents a significant step forward in understanding cosmic phenomena and promises continued contributions to the field.

A novel machine learning approach for timing characterization of gamma-ray events

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Abstract

Pulse analysis of detected radiation plays a significant role in all aspects of nuclear physics. Time-of-arrival information of the detected radiation is crucial in applications ranging from nuclear state lifetime measurements to certain medical imaging modalities such as time-of-flight (TOF) PET. In this sense, one of the top-performing algorithms for precise timing characterization is the well-established constant fraction discrimination method (CFD). In recent years, the use of machine-learning (ML) techniques has shown its potential to further improve the CRT achieved by standard methods. However, ML techniques rely mostly on improving resolution by training on a detector-pair basis. In the case of a scanner with hundreds of detectors, this approach would require optimizing too many possible models. In this work, we propose a ML timing model which can be trained for each detector individually, increasing the robustness and flexibility of this approach.

In this work we used data acquired with ^{22}Na and ^{60}Co point sources using a pair of conic 2" $\text{LaBr}_3(\text{Ce})$ detectors connected to Hamamatsu R9779 PMTs sampled at 5Gs/s, for which coincidence resolving time (CRT) of 150 ps are typically achieved using the CFD method. The detectors were set in coincidence mode, and the sources were placed at different positions between the detectors. 150000 and 200000 events respectively were acquired in total. A fully-connected dense neural network model was trained with the events of each detector. Once the models were trained, the TOF was determined from the difference between the time assigned to each event by each model. An average of 160 ps coincidence resolving time (CRT), similar to the CFD method was achieved. These promising initial results are expected to be improved with better ML models, but they already provide an efficient alternative way to analyze the timing of pulses in nuclear physics.

The TRITIUM Project: an in-water tritium monitor in quasi-real time for NPPs.

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Abstract

Large amounts of tritium are produced in the water cooling system of NPPs and released into the environment. The European directive 2013/51/Euratom establishes the tritium limit for drinking water in Europe at 100 Bq/L. As no commercial instrument is able to measure the tritium activity in water in quasi-real time, the TRITIUM project, funded by the Interreg-SUDOE program in the 2016 call, has as goal to develop such a device. An increase in the tritium activity released could indicate a malfunctioning of the reactor. The TRITIUM project aims to develop a monitor based on solid scintillators with an activity detection limit in quasi-real time of at most 100Bq/L. The TRITIUM project is a consortium composed of the University of Extremadura, the University of Aveiro, the University of Valencia, the CNRS (France) and the Junta of Extremadura (The authority for the Almaraz NPP).

The TRITIUM detector consists of a bundle of scintillating fibres in contact with the water sample which detects the tritium decay electrons. These fibres are read out by photosensors (SiPMs or PMTs for the various prototypes). SiPMs arrays have a number of advantages such as compactness, robustness,, large efficiency for photon detection and low working voltage, crucial for a monitor running without supervision but need to correct for their variation of gain with temperature A water purification system prepares the water sample before introducing it into the detector for tritium measurement. A cosmic veto and passive lead shielding reduce the natural radioactive background of the detector which otherwise would be of the order of the count rate to be measured.

A prototype is presently installed in the Arrocampo damm monitoring site of the Junta of Extremadura Simulations carried out with the Geant4 code indicate that with 5 TRITIUM modules an MDA lower than 100 Bq/L could be reached.

Nuclear structure studies of heavy and superheavy elements through mass measurements at SHIPTRAP

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The SHIPTRAP collaboration

Abstract

Mass measurements are a valuable tool to study nuclear structure [1]. Through the measurement of atomic masses, nuclear binding energies are directly obtained, enabling the study of the shell structure evolution, and locations and strengths of shell closures. Furthermore, with sufficiently high mass resolving power, direct measurements of the excitation energies of low-lying, long-lived isomeric states become possible.

The goal of the SHIPTRAP experiment, placed downstream from the SHIP separator at GSI Darmstadt, is to study heavy and superheavy nuclei produced via fusion-evaporation reactions [2]. These nuclei are very interesting from the nuclear-structure point of view, testing and improving our understanding at the highest proton numbers. However, they are particularly challenging to study due to their extremely low production rates, as low as a few detected particles per day. The high sensitivity and precision of the double Penning trap mass spectrometer SHIPTRAP are key to enable these measurements.

In this contribution, the SHIPTRAP setup and measurement technique will be introduced, and selected highlight results will be presented.

[1] J. Dilling et al, Annu. Rev. Nucl. Part. Sci. 68, 45-74 (2018)

[2] F. Giacoppo et al, Acta Phys. Pol. B 48(3) 423-429 (2017)



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