
DIPC 2021
Donostia International Physics Center

ON THE COVER THE COSMIC WEB

Matter in the Universe is arranged as a collection of large voids, filaments, and knots. These structures, which can span millions of light-years across, are collectively referred to as the cosmic web and it is the result of the nonlinear gravitational interaction of dark matter and baryons in an expanding Universe accelerated by dark energy. Supercomputers simulations are essential to understand the emergence of such structures by following the evolution of inhomogeneities in the primordial Universe and their relation to fundamental physics in nature.

The cover shows the distribution of matter in the Universe, as predicted by a supercomputer simulation that follows near one trillion resolution elements. Empty regions are shown in light blue whereas high-density regions are displayed in yellow shades. These are the locations where galaxies, like our own Milky Way, are expected to form.

Image The bacco simulations | Raul Angulo

The BACCO simulation project: exploiting the full power of large-scale structure for cosmology
Angulo RE, Zennaro M, Contreras S, Arico G, Pellejero-Ibanez M, and Stucker J.Monthly Notices of the Royal Astronomical Society 507, 5869 (2021).

2021

DIPC ACTIVITY REPORT

Science for Society

The global crisis provoked by the spread of the Covid-19 virus has clearly shown the necessity of developing advanced science to confront social challenges. The incredibly rapid development and approval of vaccines against the Covid-19 has been built on a reservoir of sophisticated knowledge developed, in general, for completely different purposes. A large part of the research results on messenger-RNA that triggered the generation of the Pfizer-BioNTech and Moderna vaccines, for instance, came from the field of immunotherapy and oncology research. This is a paradigmatic example of how basic science often finds its practical application in unexpected circumstances and fields.

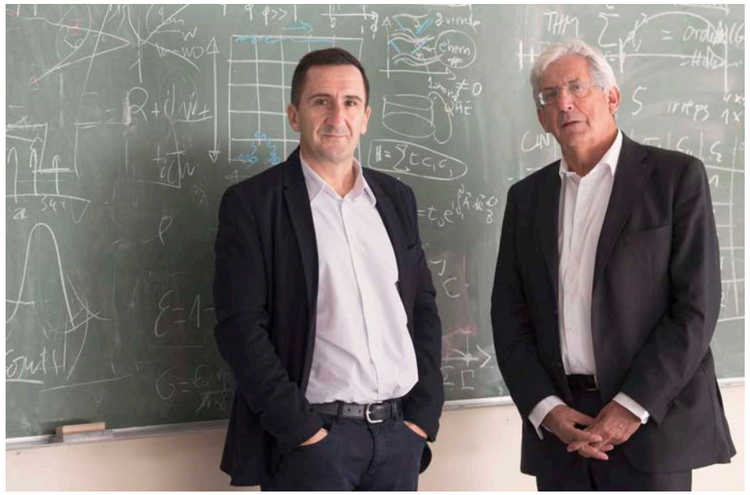
Modern societies are open, complex, and internationally interconnected.

They evolve very quickly. Continuous mutations lead to new dilemmas. As a society, we need to be prepared to face and hopefully overcome future and still unknown difficulties. We will also need to embrace novel technological advances arriving in the near future and learn how to benefit from them. A way to do this is by increasing our general arsenal of knowledge, covering a spectrum of disciplines as wide as possible.

This is our mission at DIPC. We are a research center that performs frontier research in physics and related disciplines. Scientific activity at DIPC addresses fundamental topics that take place on very different length and time scales, from elementary particles to atoms, nanostructures, mesoscopic systems, and galaxies. Scientists at DIPC work on topics such as condensed matter physics, advanced materials, quantum technologies, chemical physics, computational chemistry, photonics, photochemistry, polymer physics, biophysics, cosmology, astrophysics, and particle physics, to name a few. Let us emphasize that each one of the research lines mentioned above is not an isolated system. These research areas are open systems with blurry borders and extremely interesting projects can arise at their intersections. This is an approach that we encourage at DIPC. DIPC provides a creative and stimulating atmosphere that fosters the exchange of ideas among researchers and the blending of innovative research paths. Collaboration among scientists with different backgrounds helps to address problems with a higher degree of complexity.

In spite of the difficulties that the pandemic brought to the global science community, 2021 has been an excellent year for DIPC. Our scientists published more than 430 scientific articles and DIPC articles received roughly 24,000 citations in 2021. One might be tempted to see these numbers as just numerical indicators. They are not. There is an enormous amount of new knowledge created in such a large number of scientific articles.

An important part of our mission at DIPC is to share science with society. This is not restricted to the diffusion of some of the last scientific discoveries to the general public. DIPC's Science Communication program transmits how science is developed on a daily basis. It humanizes the scientists and establishes connections to other branches of knowledge and culture. Science cannot and should not be divided from the general body of human culture. We are convinced that the development of scientific culture helps to spread free and critical thinking in society.



Ricardo Díez Muiño, Director of DIPC and **Pedro Miguel Echenique**, President of DIPC

The activity of DIPC in 2021 was only possible thanks to the commitment, effort, and enthusiasm shown by all scientific, technical, and administrative members of the DIPC community. They are indeed the main protagonists of the success of the center.

DIPC is an inclusive and international center. It gathers scientists from all over the world because we consider science to be a collective endeavor. It benefits from diverse perspectives. These last days, due to the military invasion of Ukraine, we are witnessing a war in Europe that defies any previous expectation. As already stated in an institutional statement, we would like to express our support to those in our local scientific community suffering from this situation. We extend our sympathy to their families, relatives, and friends and hope that our scientific community and institutions will contribute to our common goal: peace. ■

Donostia International Physics Center (DIPC) is a research center opened in the year 2000. DIPC's mission is to perform and catalyze research in physics and related disciplines, as well as to convey scientific culture to society. DIPC is a foundation in which both public institutions (Basque Government, Gipuzkoa Provincial Council, Donostia/San Sebastian City Council, and the University of the Basque Country) and private companies (currently Kutxa, CAF, Telefónica, and EDP) participate and contribute to its funding. In 2008, DIPC was awarded the distinction of Basque Excellence Research Center (BERC) by the Basque Government's Department of Education. In 2019, DIPC was recognized as a Severo Ochoa Center of Excellence by the Spanish Ministry of Science and Innovation.

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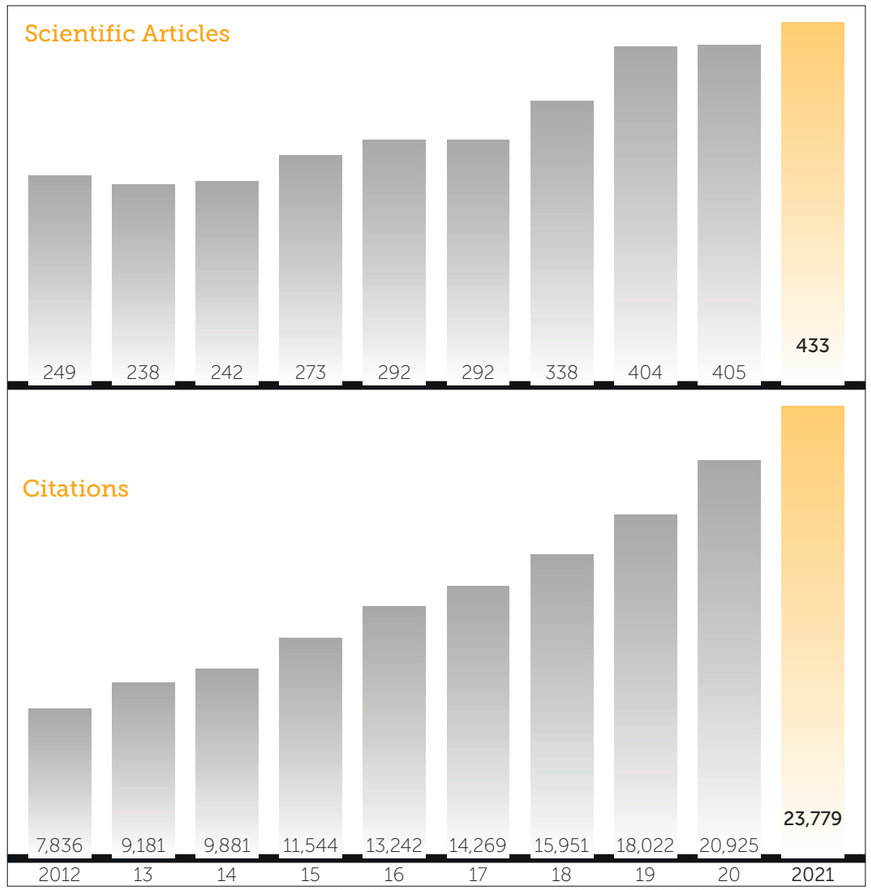
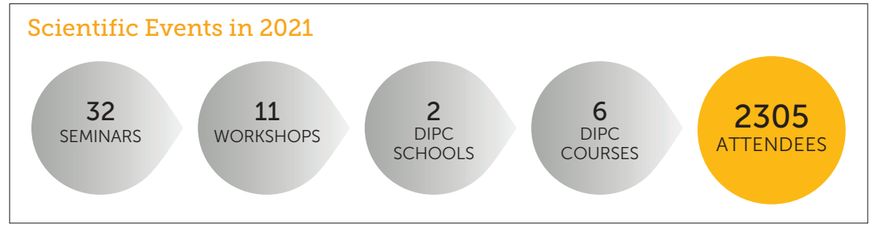
Research Activity at a Glance

After an arduous year due to constraints associated to the Covid-19 pandemic, DIPC's scientific production and its international impact has started to grow again. In 2021, **433 scientific articles** were published. That's 7% more than during 2020. In the last 23 years, the Center has published a total of **4,845 ISI publications** and has received more than **178,600 citations**.



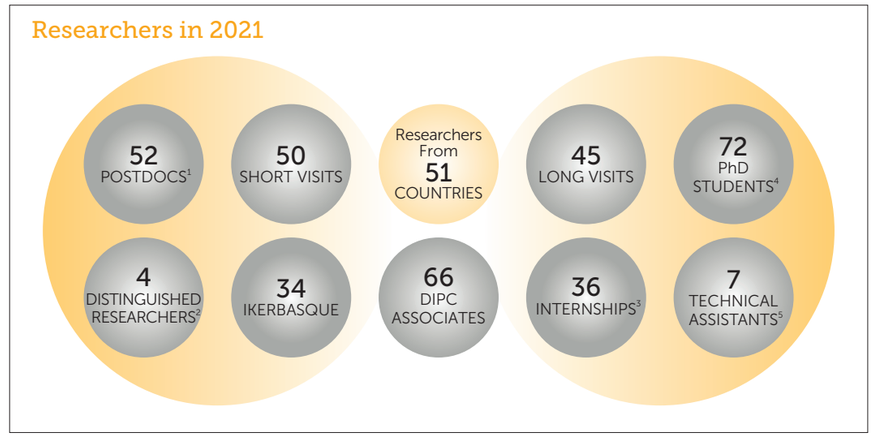
Source Web of Science Core Collection (all years and all indexes, 03/03/2022)



In addition to doing research, DIPC's annual strategic agenda of actions foster exchange with scientists from around the world. Our Scientific Events include several formats. Seminars, given by international experts, cover research topics of particular interest to our community. Our Workshops highlight specific subjects of interest. And both the DIPC Schools and the Courses, especially aimed at young researchers, focus on learning particular skills. Even though during 2021 some in person activities were resumed, most of the programmed events were still held online.

Driving Force of DIPC's Research Activity: Our Highly Dynamic Community

The core of the DIPC Community is made up of local scientists as well as PhD students and postdoctoral researchers who come from other institutions. They complete their training and hone their expertise with us. DIPC Associates are situated in other centers at different faculties of the University of the Basque Country and the Materials Physics Center. Our scientists act as hosts for a generally large number of international visiting researchers and subsequently acquire their shared knowledge. This helps to develop our long-term DIPC research projects. Among the local host community, there are also Ikerbasque Researchers, who play an important role. Fortunately, during 2021, DIPC's international visitors program resumed after having been cancelled in 2020 following the public health authorities' recommendations.

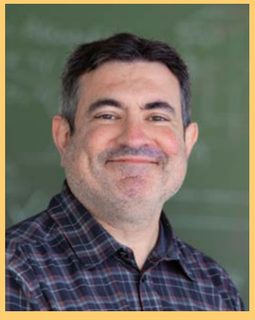


[1] Postdoctoral Positions and Research Collaborators. [2] Distinguished Researchers and Fellows.
[3] Internships and Undergraduate Students. [4] PhD Students and Research Assistants. [5] Technical Assistants and Engineers.

DIPC Supercomputing Center

The Supercomputing Center at DIPC is its great strategic infrastructure and serves as a fundamental tool for the excellent research carried out by our researchers and those of other research centers in the Basque Country

Computational physics and chemistry are among the strongest research fields in the Basque Country and the Supercomputing Center is one of its key resources. In recent years the Supercomputing Center has also started offering its services to other type of research lines related to Cosmology, Genetics, Artificial Intelligence, Mathematics... With its current level of physical, human and technical resources this high performance computing (HPC) center has become a focus of technological knowledge, training, and innovation. Its status and influence transcend its primary mission, not only as a tool but also as a discipline in itself. There is no more powerful computing center of its type in the Basque Country.



"The variety and power of the computing resources of DIPC, and its constant upgrade, allow the permanent confrontation of a wide range of numerical simulations that put DIPC and other research centers of the Basque Country at the forefront in research"

Txomin Romero Asturiano
Director of the DIPC Supercomputing Center

Current computing resources

The Center has two rooms to host the HPC systems. These rooms have an isolated electrical connection, communications infrastructure, humidity, electricity consumption and temperature control sensors, various uninterrupted power supply systems, refrigeration systems, automatic fire-extinguishing systems and intrusion detection.

As of 2021, the Center has several supercomputers covering a wide range of computational needs. Its main facility is the supercomputer ATLAS, a cluster with Xeon nodes (from 24 cores and 128 GB of RAM small nodes to large shared memory nodes with 52 cores and 1.5 TB of RAM in a single operating system image). With more than 10,000 cores and 80 TB of RAM, ATLAS is one of the most powerful supercomputers in Spain. In addition, some of our supercomputers have NVIDIA Tesla P40 and GeForce RTX 3090 technology for GPGPU programming, Xeon Phi technology and ARM and AMD processors based nodes.

TOTAL FIGURES

10,723 cores

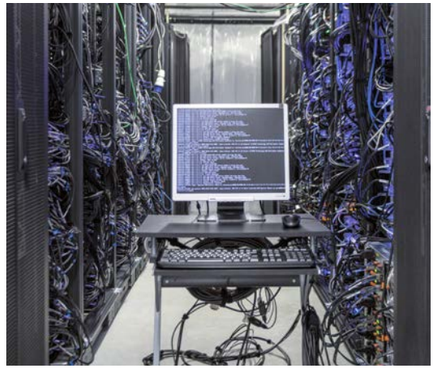
82 TB of RAM

346 TB of scratch disks

832 TB for home directories

Non-stop service: 24 hours 365 days

About 400 researchers from DIPC and other research centers of the Basque Country such as the UPV/EHU, the CSIC-UPV/EHU Materials Physics Center, CIC nanoGUNE, CIC Biomagune, IIS BioDonostia, several BERCs (like BCAM, BCBL, BCMaterials, Biofisika, Achucarro or BC3) and Ikerbasque used this computational infrastructure in 2021.



Science Communication

One of the pillars of DIPC is Science Communication, a task that we enthusiastically carry out to transfer scientific knowledge to society. We are therefore particularly pleased to have been able to bring back our extensive outreach program in its entirety in 2021. In compliance, of course, with health regulations and capacity reductions, we have organized **79 events** with the direct participation of more than **23,000 people**, both in person and online. Those events had more than **35,000 views** from various media outlets. We are delighted to see that people have continued to respond to our educational and cultural offerings with passion.

ZIENTZIAKUTXA / The Traveller Gene

Kutxa Fundazioa and DIPC have been organizing a program of dissemination talks aimed at the general public for many years. In 2019 it materialized in the series of talks *ZientziaKutxa*.

After the jump to the online format in 2020, the program was revived under the slogan "The Traveller Gene" in a hybrid format so that people could attend in person or follow it online. This new edition honored our most adventurous scientists, and brought together prestigious scientists with a traveling and explorer profile to contemplate the world with new eyes, with a new scientific perspective.

This series of public lectures, in Basque and Spanish, were scheduled during June and July with reduced capacity and they were attended overall by 297 people. All the content and audiovisual material created within Zientziakutxa is available on our Youtube channel and accumulates thousands of views.

02/06/2021
Kutxa Kultur Plaza, Tabakalera
Pirinioak, mendien ikuskizun geologikoa
Asier Hilario Geologist
Euskal Kostaldeko UNESCO Geoparkea,
International Union of Geological Sciences

23/06/2021
Kutxa Kultur Plaza, Tabakalera
XIXgarren mendeko belaontzi batean bizi, esploratu eta ikertu
Maria Intxaustegi Underwater Archaeologist
UPV/EHU, Bark Europa,
Alegria Expediciones, Ondaresub

07/07/2021
Kutxa Kultur Plaza, Tabakalera
El cambio climático y los polos. Expediciones a los hielos
Jerónimo López Geologist
Universidad Autónoma de Madrid (UAM),
Scientific Committee on Antarctic Research (SCAR)

Jerónimo López in his talk about climate change accompanied by Ricardo Díez Muiño.

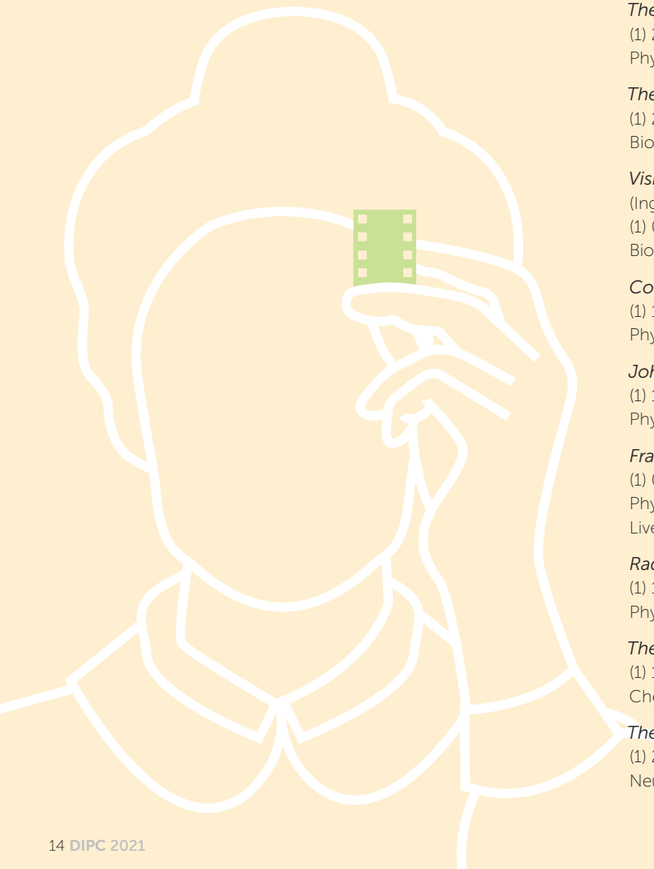
28/07/2021
Eureka! Zientzia Museoa
Astronomía para el desarrollo en África: un viaje de 15 años entre dos pasiones
Mirjana Povic Astrophysicist
Ethiopian Space Science and Technology Institute (ESSTI), Instituto de Astrofísica de Andalucía (IAA-CSIC)

CINEMA AND SCIENCE

The Basque Film Archive, Donostia International Physics Center (DIPC) and the San Sebastian International Film Festival (SSIFF) organized in 2021 the fourth edition of 'Cinema and Science' with the objective of transmitting film culture and scientific culture. The cycle took place from January to March 2021, in Tabakalera, in Donostia/San Sebastián, and the Fine Arts Museum in Bilbao. Always seeking to stimulate connections with different scientific fields, the 10 films screened in both towns were preceded, as is tradition, by inspiring presentations and subsequent discussions led by prestigious scientists.

The Covid-19 pandemic, and its impact in our daily life, came to reaffirm the principles 'Cinema and Science' stands for: greater scientific culture helps us as a society to take better, well-grounded decisions and, as André Malraux taught us, a greater cinematographic culture makes us inheritors of the nobility and beauty of the world.

In this edition we could finally enjoy the screening of ***Woman in the Moon*** (Fritz Lang, 1929) with live music by Javier Pérez from Azpeitia. Screenings foreseen at Le Select cinema in Saint Jean de Luz had finally to be cancelled due to cross-border restrictions related to pandemics.



General Sessions

Films projected in
Donostia/San Sebastián (1) and Bilbao (2)

The Man Who New Infinity (Matt Brown, 2015)
(1) 08/01/2021 (2) 09/01/2021
Physicist **Pedro Miguel Echenique**, UPV/EHU, DIPC

The imitation game (Morten Tyldum, 2014)
(1) 22/01/2021 (2) 23/01/2021
Physicist **Aitzol García Etxarri**, DIPC, Ikerbasque

The Savage Innocents (Nicholas Ray, 1960)
(1) 28/01/2021 (2) 30/01/2021
Biologist **Juan Ignacio Pérez Iglesias**, UPV/EHU, DIPC

Viskningar och rop / Cries and Whispers
(Ingmar Bergman, 1972)
(1) 04/02/2021 (2) 06/02/2021
Biochemist **María Muñoz Caffarel**, Biodonostia, Ikerbasque

Contagion (Steven Soderbergh, 2011)
(1) 11/02/2021 (2) 13/02/2021
Physicist **Itziar Pérez Irazusta**, Osakidetza

Johnny got his gun (Dalton Trumbo, 1971)
(1) 19/02/2021 (2) 20/02/2021
Physicist **Javier Aizpurua**, CFM (CSIC-UPV/EHU), DIPC

Frau im Mond / Woman in the Moon (Fritz Lang, 1929)
(1) 05/03/2021 (2) 06/03/2021
Physicist **Ane Sarasola**, UPV/EHU, DIPC
Live music by pianist **Javier Pérez de Azpeitia**

Radioactive (Marjane Satrapi, 2020)
(1) 12/03/2021 (2) 13/03/2021
Physicist **Maia García Vergniory**, DIPC, Ikerbasque

The Andromeda Strain (Robert Wise, 1971)
(1) 19/03/2021 (2) 20/03/2021
Chemist **Fernando Cossío**, UPV/EHU, Ikerbasque

The Miracle Worker (Arthur Penn, 1962)
(1) 25/03/2021 (2) 27/03/2021
Neurophysiologist **Xurxo Mariño**, Universidade da Coruña

Scholar Sessions

The film selected for the scholar sessions was "***The imitation game***" (Morten Tyldum, 2014), a biopic about the British mathematician Alan Turing, famous for having deciphered the secret Nazi codes contained in the Enigma machine, decisive in the final outcome of the second world war. Turing is considered the father of artificial intelligence. Instead of being recognized as a hero, he was persecuted because of being homosexual. In order to give a broad vision on the film, experts in computer science and scientists involved in equality and diversity issues were invited to participate in the presentations.

Finally, the events scheduled at the Fine Arts Museum of Bilbao could be celebrated but those in San Sebastian were cancelled due to pandemics:

16/02/2021
Bilbao Fine Arts Museum
Imitazio Jokoa (In Basque)
Olatz Arbelaitz Computer Scientist from UPV/EHU
Aitzol García Etxarri Physicist from DIPC, Ikerbasque

16/03/2021
Bilbao Fine Arts Museum
El dilema Turing (In Spanish)
Ignacio Arganda-Carreras Computer Scientist from UPV/EHU, Ikerbasque
Idoia Mujika Chemist from CFM (CSIC-UPV/EHU)

José Luis Rebordinos (Director of the San Sebastian International Film Festival), Pedro Miguel Etxenike (President of DIPC), Joxean Fernández (Director of the Basque Film Archive), Ricardo Díez Muiño (Director of DIPC), Edurne Ormazabal (General Director of Tabakalera) and Miguel Zugaza (Bilbao Fine Arts Museum Director) in the presentation of the Cinema and Science Cycle.

WOMEN IN SCIENCE

08-28/02/2021

In 2021, 11 science institutions joined forces at *Emakumeak Zientzian* to present a common program on the occasion of the **International Day of Women and Girls in Science** that is celebrated the 11th of February worldwide. This alliance was integrated by DIPC, CIC nanoGUNE, the Materials Physics Center (CFM CSIC-UPV/EHU), CIC biomaGUNE, Biodonostia, Tecnun, Ceit, POLYMAT, Elhuyar, the Faculty of Informatics of the University of the Basque Country (UPV/EHU) and Eureka! Zientzia Museoa.

Emakumeak Zientzian initiative offered a complete program of activities in Donostia/San Sebastián throughout February. The objective of the program is making the activity of women in science visible, breaking with the typically male roles attributed to scientific-technical activities, and encouraging the choice of scientific careers among girls and teenagers.

This year *Emakumeak Zientzian* grew enormously, partly thanks to the adherence of new entities and partly to the hybrid format adopted (face-to-face and virtual), multiplying by more than four the direct participation with respect to the previous year, reaching a total of 2,410 people.

17 activities aimed at all audiences, including workshops, public talks, family experiments and virtual visits were put together thanks to this highly cooperative alliance:

08-28/02/2021 | Eureka! Science Museum
Mujeres en Ciencia Exhibition
General public

11/02/2021 | Tabakalera
13/02/2021 | Fine Arts Museum from Bilbao
Cinema and Science: «Contagion» screening presented by Itziar Pérez (Osakidetza)
General public

12/02/2021 | Eureka! Science Museum,
Live and streamed
Women scientists from yesterday and today Public lecture
General public

Invited scientists and honored scientists:
Fátima Villa Tecnun, **Neri Oxfam**
Ester Verde CFM CSIC-UPV/EHU, **Carmen Mijangos**
Naiara Aginako Bengoa UPV/EHU, **Hedy Lamarr**
Ane Ruiz de Angulo CIC biomaGUNE, **Gertrude Belle Elion**
Elisa Jimenez UPV/EHU, Ikerbasque, DIPC, **Rachel Carson**

The event featured live music by:
Ane Leux and **Tineke van den Berg**

16/02/2021 | CIC biomaGUNE
Virtual tour of CIC biomaGUNE Streaming
General public

17/02/2021 | Biodonostia
Learn how to diagnose Covid-19 Streaming
1-4 Secondary School

19/02/2021 | Tecnun
Playing at being an engineer Workshop
3-4 Secondary School

20 and 21/02/2021 | Eureka! Science Museum
The stars of science, tribute to women in science Hands-on experiments
For families (ages +6)

22 and 25/02/2021 | Science Computing Faculty UPV/EHU
Coding of tale and magic Streaming
4-6 Elementary School

23/02/2021 | DIPC and CFM
Virtual tour of DIPC and CFM Streaming
3-4 Secondary School and High School

25/02/2021 | CIC biomaGUNE
Encounter with CIC biomagune female researchers Streaming
5 Elementary School

Online Resources | CIC nanoGUNE and Polymat
Science is indeed a girls thing
Hands-on experiments on nanoscience and polymers science

Online Resources | Biodonostia, CIC biomaGUNE; DIPC and CFM
The power of experience
Hands-on experiments to empower adult women as transmitters of scientific culture

For more information visit
https://**emakumeakzientzian**.eus

PRIDE IN SCIENCE

For the third year since 2019 and under the slogan *"Harrotasuna Zientzian / Orgullo en Ciencia"* (Pride in Science), CIC nanoGUNE, the Materials Physics Center (CFM CSIC-UPV/EHU) and DIPC jointly commemorated the **International Day of Pride in STEM** which is celebrated internationally the 18th November. The initiative aims to give visibility to the LGBTQIA+ collective in science, actively contribute to break old stereotypes and to celebrate diversity as a pillar in the future of science.

To celebrate Pride in Science Day 2021, we launched a social media campaign to highlight LGBTQ scientists working in our centers. The goal was to generate new role models for future generations of scientists and to show that our centers are safe spaces for the collective also to our own community. PhD students, Post-doctoral researchers and STEAM professionals kindly accepted our invitation to participate in the awareness-raising campaign.

MESTIZAJES

Mestizajes is a project aimed at all audiences designed under an innovative and original perspective to foster dialogue between science, literature and humanities. The project is promoted and organized by DIPC within the framework of Euskampus and coordinated by Gustavo Ariel Schwartz. Different activities such as conferences, seminars, presentations or collaborative projects have been carried out in collaboration with San Telmo Museum, Donostia Kultura, Tabakalera and the Vice Rectorate of the Guipúzcoa Campus of the University of the Basque Country (UPV/EHU).

In 2021, the International Conference on Literature and Science was organized in San Sebastian, including two programmed activities: an academic workshop at DIPC in the morning and a cycle of open public lectures at Tabakalera in the afternoon.

22-24/11/2021
Donostia/San Sebastián
International Conference on Literature and Science

The *IV Meeting on Literature and Science – A trans-disciplinary approach to beauty from Science, Art and Literature* was focused on issues that have to do with beauty, aesthetic perception and its relevance in Art, Literature and Science from multiple perspectives.

What happens in our brain when we appreciate something beautiful? Can science help us understand beauty? Are there universal principles for aesthetic appreciation? These and other questions where addressed in this stimulating encounter between scientists, writers and artists in order to explore a broader vision of the world, science and culture.

Public Lectures Tabakalera
Invited speakers and public lectures:

22/11/2022
Bello como el cálculo improbable de una danza de estorninos
Francisco González Universidad de Oviedo

Una poética del Carbono 14
Luisa Etxenike Writer

23/11/2021
¿Por qué la ciencia necesita al arte?
Elisa Garrido Universidad Autónoma de Madrid

La falacia de lo natural
Agustín Fernández Mallo Writer

24/11/2021
¿En qué se parecen la mecánica cuántica y la literatura?
María García Díaz Universitat Autònoma de Barcelona

La verdad y la belleza de las estructuras literarias
Javier Argüello Writer

For more information visit
www.**mestizajes**.es

ON ZIENTZIA

On Zientzia video competition, organized annually by DIPC and Elhuyar in the framework of the television program *Teknopolis*, has the goal of producing and disseminating short and original videos on science and technology, aimed at all audiences.

For its eleventh edition, a total of 86 works were received, with gender balance among the participants. Videos have been submitted in Basque, Spanish and English from all over the world, including Basque Country, Spain, Germany, the United Kingdom, Mexico and Peru, among other countries.

The 2021 awards ceremony was held on June 15 at Tabakalera.

BEST DISSEMINATION VIDEO
¿Por qué no podemos tomar un ibuprofeno cada 4 horas pero sí alternarlo con paracetamol?
Yasia Dolisnea

Deepfake, etorkizuna atarian
Unai García, Mikel González, Eneko Mosquero and **Alex Bouza**

YOUNG PRIZE
Aurrera goaz
Urdinak & Berdeak secondary school students Toki Alai school, Irun

SPECIAL MENTION
Ciencia
Carmen Reja Aexpainba, Badajoz

For more information visit
www.**onzientzia**.tv

SESSIONS FOR KIDS
San Sebastian International Film Festival

17-25/09/2021
Belodromoa Ikastetxeetan, School premises

For the third year, the San Sebastian International Film Festival (SSIFF), DIPC and the Basque Film Archive organized film sessions for schools to connect two of the city's hallmarks: its passion for cinema and its high specialization in science. The chosen title for 2021 edition was ***Tadeo Jones 2: Midas erregearen sekretua*** (Tadeo Jones 2: The Secret of King Midas). Thousands of schoolchildren from Gipuzkoa, between ages of 6 and 11 years, were able to enjoy the film dubbed into Basque for the occasion. Due to the Covid-19 pandemic, the velodrome couldn't be used as a giant film theatre for the second year in a row. However, as the previous year, the screenings for schoolchildren were held in the classrooms, maintaining the spirit of making science more accessible through cinema. The activity, renamed ***Belodromoa ikastetxeetan***, included a video lecture by the underwater archaeologist ***Maria Intxaustegi***, who introduced the film and talked about her experience investigating the underwater heritage all over the world. An estimated of 14,500 students from 50 schools enjoyed the lecture and the screening.

MARS IN LIVING COLOR

To commemorate an important milestone in space exploration of the red planet, the arrival of NASA's Perseverance rover to Mars, we organized a public online event bringing together different actors of the space missions to Mars. For the occasion we featured Carrie Bridge, a scientist at NASA and chief of scientific operations team of the Mars rover Curiosity, as well as the leaders of the Basque participation in the rover Perseverance of the MARS2020 mission, the UPV/EHU professors Agustín Sánchez-Lavega and Juan Manuel Madariaga, and the CEO of AVS, the engineering company from Elgoibar with presence on Mars, Miguel Ángel Carrera. All the lectures and colloquia were introduced and moderated by the astrophysicist and Ikerbasque researcher at DIPC, Silvia Bonoli and simultaneous translation was offered to three languages (Basque, Spanish, English). 100 people attended the event online and it has accumulated hundreds of visualizations.

Introduction
El planeta rojo
Silvia Bonoli DIPC and Ikerbasque

Part 1: CURIOSITY
Roving on Mars: Curiosity's Journey, Discoveries and Next Adventures
Carrie Bridge NASA JPL, California (USA)

Part 2: PERSEVERANCE MARS2020
La atmósfera de Marte
Agustín Sánchez-Lavega Planetary Science Group UPV/EHU

La Exploración de Marte desde la perspectiva de la Química Analítica: el instrumento SuperCam y la Misión NASA-Mars2020
Juan Manuel Madariaga
IBeA Analytical Research and Innovation Group UPV/EHU

Presente y futuro de AVS en Marte
Miguel Ángel Carrera AVS Added Value Solutions

ARANZADI ASTRONOMICAL DAYS

07-08/10/2021
Z hall, Tabakalera

In 2021, for the first time DIPC collaborated in the organization of the 30th edition of Aranzadi Astronomical Days. The program included lectures on astrophysics and cosmology from two DIPC researchers, as well as the special participation of José Carlos del Toro from the Institute of Astrophysics of Andalucia (IAA-CSIC).

07/10/2021
Unibertsoaren historia laburtua: 14.000 milioi urte ordu laurdenean
Lurdes Ondaro DIPC

¿Deberíamos adorar todos a la gran araña cósmica?
Marcos Pellejero DIPC

El Sol: 54 añitos en una historia de 4500 millones
José Carlos del Toro Iniesta
Institute of Astrophysics of Andalucia (IAA - CSIC)

08/10/2021
Espectropolarimetría solar desde el espacio
José Carlos del Toro Iniesta Institute of Astrophysics of Andalucia (IAA - CSIC)

SCIENCE AND CHESS: INFINITE CONNECTIONS

09-11/10/2021
Eureka! Zientzia Museoa

The relationship between chess, science, education, and art, as well as the role of women in this ancient game, were some of the topics addressed during **Science and Chess: Infinite Connections**, a tree-days encounter organized by DIPC and Eureka! Zientzia Museoa.

The event brought together distinguished guests from the world of chess, science research, photography, literature and education, to discuss on the surprising links between these disciplines. More than 1,600 people participated directly in the programmed lectures and round tables.

Chess fans were able to enjoy simultaneous chess sessions with Grandmaster (GM) Miguel Illescas and Women Grandmaster (WGM) and International Master (IM) Olga Alexandrova, as well as a Blitz Tournament, both organized in collaboration with the **Gros Xake Taldea** chess club.

09/10-28/11/2021
The Thinkers Photographic Exhibition
David Llada Chess photographer, FIDE

09/10/2021
Artificial Intelligence and chess Public Lecture
Miguel Illescas Grandmaster (GM)

Chess and reality Public Lecture
Diego Rasskin Biologist and writer, Universidad de Valencia

The Thinkers Public lecture
David Llada Chess photographer, FIDE

The role of women in chess Open interview
Olga Alexandrova (WGM & IM)

Triangulating Chess: Science, Art and Society Round table
Miguel Illescas (GM), **Olga Alexandrova** (WGM & IM), **Diego Rasskin**, and **David Llada**

10/10/2021
Simultaneous Chess Sessions
Miguel Illescas (GM) and **Olga Alexandrova** (IM)
Organized by Gros Xake Taldea

Chess and science: the view of an amateur Public Lecture
Paola Ferrario Physicist, DIPC

Chess teaches to think Public lecture
Leontxo García Chess journalist

11/10/2021
Blitz Tournament
Organized by Gros Xake Taldea

Grandmaster Olga Alexandrova playing chess with members from Gros Xake Taldea.

JOT DOWN 2021

03/12/2021
Tabakalera

In 2021 Jot Down was held for the first time in San Sebastian organized by the well-known magazine Jot Down and DIPC. Previous editions have been held annually in Seville and this one too had the support of the University of Seville.

The meeting brought together some of the best known faces of science, illustration and science popularization with a dynamic program that included short talks and round tables around science and comics. The event concluded with the awarding of the prizes for the contest of popularization sponsored also by Canfranc Underground Laboratory (LSC) and Laboratorium Bergara.

Lecture
En busca del grafo perdido
Clara Grima Mathematician, Universidad de Sevilla, *Mati y sus mateaventuras*

Round table on Comic and Education
Dani Fano Cartoonist, *Anubis 3.0*
Raquel GU Cartoonist, *Mati y sus mateaventuras*
Hodei Iparraguirre Cartoonist, *nanoKOMIK*
Amaia Arregi Moderator, DIPC

Lecture
¿Por qué irnos bajo tierra para entender el origen del Universo?
Francesc Monrabal Physicist, DIPC and Ikerbasque, NEXT proyect

Round table on Comics and Outreach
Juanjo Gómez Cádenas Physicist, DIPC and Ikerbasque, NEXT proyect
Panchulei Cartoonist, NEXT proyect
Juan Manuel García Ruiz Geologist, ERC PROMETHEUS – *Algo en el agua*
Ángel Fernández Moderator, Jot Down

Retos y futuro de la ilustración científica
Vega Asensio Biologist and Illustrator, NorArte Estudio

Jot Down 2021 Science Outreach Contest Award Ceremony

Best Popular Science Essay Award
Los espectadores | **Charo Sabariegos Jareño** Professor of Microbiology, University of Albacete

Best Science Fiction Narrative Award
Dentrofueradentro | **Javier Izcue Argandoña** Language and Literature teacher

Best Scientific Illustration Award
Sinergia | **Alfonso Barragán** Designer

ANIMAL ADAPTATION, EVOLUTION AND NATURE
Presentation and Colloquium

08/04/2021
San Telmo Museum, Donostia/San Sebastián

The recently published book ***Animales ejemplares*** (Next Door, 2020) with texts by biologist Juan Ignacio Pérez Iglesias and illustrations by Yolanda González was presented in San Sebastian in an event organized by DIPC and the Chair of Scientific Culture of the University of the Basque Country (UPV/EHU) with the collaboration of San Telmo Museum.

Taking the text of the book as a starting point, its author, professor of physiology, reflected on animal adaptation, evolution and nature, conversed with Arantza Etxeberria, expert in the philosophy of biology and medicine, and Ander Izagirre, writer and journalist, and a great connoisseur of a wide variety of natural landscapes.

The colloquium served to highlight the versatility of animal nature, and the great capacity of animal organisms to adapt to very adverse environments. The risk of loss of a rich natural heritage threatened by human activities was also addressed in the colloquium.

Speakers
Arantza Etxeberria Professor of Philosophy of Science UPV/EHU
Ander Izagirre Journalist and Writer
Juan Ignacio Pérez Iglesias Professor of Physiology at the UPV/EHU and Director of the Chair of Scientific Culture UPV/EHU and DIPC associate

HIGH SCHOOL VISITS

Since 2014, DIPC and the Materials Physics Center (CSIC-UPV/EHU) organize visits for high school students with the objective of inspiring scientific vocations and showing our daily activities. In 2021, visits were adapted to a virtual format in which we continued introducing our research and showing different laboratories. A total of 797 students participated from 23 high schools and a special visit was scheduled within the Egokitu program of UPV/EHU.

MEETING WITH MIRJANA POVIC AND PHD STUDENTS

28/07/2021
DIPC headquarters

In this informal encounter addressed to female scientists starting their careers (Undergraduates, PhD students, Pot-docs) we had the opportunity to let us inspire by Mirjana´s exceptional scientific career, and to talk about astronomy, and the role of women in science, as well as to learn about her projects and experience in Africa. The meeting was moderated by DIPC's astrophysicist Silvia Bonoli. The activity was organized by DIPC in the framework of **Women and Science** promoted in cooperation with the Gipuzkoa Provincial Council.

Mirjana Povic is a Serbian astrophysicist working at the Ethiopian Institute of Space Science and technology (ESTI) and an associated doctor to the Astrophysics Institute of Andalucia. Her research is mainly focused on the formation and evolution of galaxies. For more than 10 years she has worked in the development of science and education in Africa, with a special focus on the role of women. In 2018 she received the inaugural Nature Research Award for Inspiring Science and in 2021 the inaugural Jocelyn Bell Burnell Inspiration Medal from the European Astronomy Society.

Donostia weekINN 2021

DIPC regularly collaborates in the Innovation Week "Donostia WeekINN" that Fomento of San Sebastian organizes every end of October. In 2021, this collaboration was renovated again through activities for both the general public and education organized in collaboration with other institutions:

18/10/2021 | Cinema and Science special screening, Tabakalera
Coherence (James Ward Byrkit, 2013)
Román Orús Lacort, DIPC Ikerbasque Professor, CEO of Multiverse Computing, and **Idoia Ochoa**, Tecnum

19/10/2021 | Aquarium of Donostia/San Sebastian
Women scientists from yesterday and today
Featuring Emakumeak Zientzian 2021 edition's speakers and honored scientists

20/10/2021 | Maker Day, touching the innovation, Kursaal
Nanoscience Workshop for schools organized jointly with CFM (CSIC UPV/EHU) and CIC nanoGUNE

SCIENCE WEEK

05-07/11/2021
Tabakalera

As every year DIPC participated along with CIC nanoGUNE and the Materials Physics Center (CFM CSIC-UPV/EHU) in the Science Week of the University of the Basque Country (UPV/EHU). The traditional stand with hands-on experiments on materials science and nanoscience was replaced this time by the organization of two special workshops.

On one hand, we organized **"Eskalatu zure mundua / Escala tu mundo"** a hands-on workshop for children focused on the experimentation of the tiny world and its visualization. On the other hand, **The Game of Brainy Roles** was a workshop for science school teachers, in which, they learned how to play with a role game that has been designed to promote scientific culture and creativity by DIPC's researcher José Ángel Martínez and María Larriva.

Lunch with all the volunteers.

06/11/2021
Eskalatu zure mundua / Escala tu mundo
Workshop for children (+6), 2 sessions

06/11/2021
The Game of Brainy Roles
Workshop for science teachers

Additionally, some of our scientists participated at **Zientzia Club**, an event within the Science Week program that disseminates science with funny monologues in a festive atmosphere:

06/11/2021
Átomos y Ordenadores
Rodrigo Menchón DIPC, UPV/EHU

Las galaxias que vemos y que nunca alcanzaremos
Daniel López DIPC

Retorcer la luz, hacer flotar objetos...y lo que no te cuentan en el colegio que puedes hacer con la física
Gabriel Molina-Terriza CFM (CSIC-UPV/EHU), Ikerbasque, DIPC

La teoría del Universoplanismo. Cuando los terraplanistas no son suficientemente ambiciosos
Marcos Pellejero DIPC

DIPC 2021 The Year in Media

106	+40	4
newspaper articles	radio impacts	television appearances

Equality at DIPC

The First Equality Plan was launched in 2020 structured in four main key areas that represent the main challenges identified during the diagnosis process: organizational culture, diversity at workforce, sexual harassment at the workplace and work-life balance.

In the first year of the plan's implementation (2020-2021), among others, we have included sex variable in administrative databases, provided our community with inclusive language guidelines and specific training was offered to the outreach personnel. In addition, a course on leadership skills was organized for early career researchers as part of the gender-sensitive empowering activities.

However, the creation and implementation of the **Protocol for preventive action and care for victims of sexual harassment and gender-based harassment, based on sexual or gender diversity** constitutes probably the most notable achievement in 2021. To this end, we counted on the expertize of Aitziber Bañuelos Ganuza from Eraikiz Kolektiboa, who has been in charge of the protocol against harassment of the University of the Basque Country (UPV/EHU). This process also included an open training for all DIPC community to raise awareness on sexual and sexist violence.

Such protocol is established to guarantee and maintain a dignified work environment for all DIPC workers, free of general violence, and violence against women and minorities, that may occur both outside and within the physical space of DIPC, as well as those that could take place through virtual or symbolic means of communication.

The body in charge of applying this protocol will be the **Confidential Advisory**, which is integrated by Beatriz Suescun, Amaia Arregi and Silvia Bonoli. They are responsible for receiving complaints or reports and their processing under the principle of confidentiality.

We will keep pushing zero tolerance policies in order to prevent harassment in our community

Additionally, DIPC has taken several actions during the last years to sensitize on gender equality and diversity in science, to make visible female and other discriminated collectives labor, to offer a wider spectrum of role models to new generations, and to break with the traditional white, heterosexual, and male stereotype of the scientist. We have become referents in the celebration of the **International Day of Women and Girls in Science** (February 11th) through the initiative ***Emakumeak Zientzian*** together with various local science institutions. Since 2019, we celebrate the **Pride in Steam Day** the November 18th along with CFM and CIC nanoGUNE. In addition, a specific program called "**Women and Science**" has been created in collaboration with Gipuzkoa Provincial Council with the main purpose of fostering the career of excellent female scientists. Finally, DIPC hosts an African researcher for several months thanks to "Science by Women" program lead by **Women's for Africa Foundation** and promoted locally in collaboration with "Gipuzkoa Coopera" by the Gipuzkoa Provincial Council. In addition, along with CFM the "Learn Africa" scholarship is offered every year to a female African student to enrol in the UPV/EHU's Master in Nanoscience.

Personnel Segregated by Sex

	Total Staff	Men	Women
Direction & Management			
Directors	4	100%	0%
Managers	4	25%	75%
Total	8	63%	38%
Scientific			
Pre-Docs	72	75%	25%
Post-Docs	52	73%	27%
Distinguished Researchers	4	50%	50%
Ikerbasque Research Fellows	7	86%	14%
Ikerbasque Research Associates	10	80%	20%
Ikerbasque Research Professors	7	86%	14%
Engineers	4	50%	50%
Technical Assistants	3	33%	67%
Total	159	74%	26%
Technical & Administrative			
Administrative Staff	10	30%	70%
IT Personnel	6	50%	50%
Outreach Personnel	2	0%	100%
Total	18	33%	67%
TOTAL	**185**	69%	31%

*Data as of 31/12/2021. Gender data are currently being collected.

Associates and Visiting Researchers

	Total Staff	Men	Women
Strategic Level			
DIPC Associates	66	76%	24%
Visiting Researchers	95	82%	18%

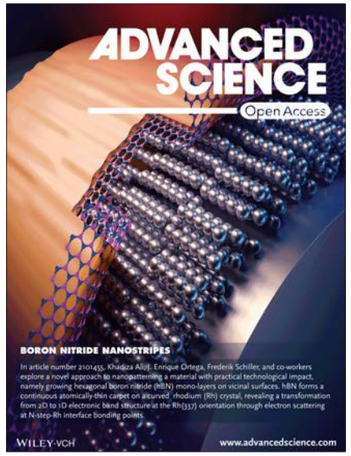
Scientific Highlights

Atomically-precise texturing of hexagonal boron nitride nanostripes

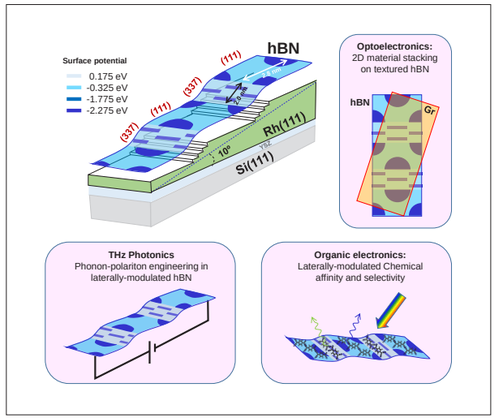
Ali K, Fernández F, Kherelden MA, Makarova AA, Píš I, Bondino F, Lawrence J, de Oteyza DG, Usachov DY, Vyalikh DV, García de Abajo FJ, Abd El-Fattah ZA, Ortega JE and Schiller F
Advanced Science 8, 2101455 (2021)

Monolayer hexagonal boron nitride (hBN) can be epitaxially grown on vicinal Rhodium (Rh) surfaces using a Rh curved crystal for a systematic exploration, which produces a periodically textured, nanostriped hBN carpet that coats Rh(111)-oriented terraces and lattice-matched Rh(337) facets with tunable width. The electronic structure reveals a nanoscale periodic modulation of the hBN atomic potential that leads to an effective lateral semiconductor multi-stripe.

Since the discovery of graphene, a wide diversity of atomic-layer-thick, two-dimensional (2D) materials with varied properties have emerged. Of particular interest are those that exhibit semiconducting behaviour, such as hexagonal boron nitride (hBN). hBN is isoelectronic to graphene and has also a honeycomb lattice formed by alternating nitrogen and boron atoms, but in contrast to the semimetallic graphene, its band structure presents some characteristics that makes it particularly attractive for applications in microelectronics, either alone or in combination with other 2D materials, such as graphene. Furthermore, hBN is structurally robust and chemically inert. Although hBN flakes may be obtained by mechanical exfoliation of bulk crystals, a single hBN monolayer can be readily synthesized on metal surfaces, leading to structurally and chemically robust substrates that frequently exhibit nanoscale patterns. This makes hBN-covered metals excellent platforms to achieve functional interfaces with atoms, molecules, and aggregates, as well as to develop hybrid 2D materials, such as twisted van der Waals stacks or 2D heterostructures. The latter hold a great potential for atomically thin circuitry, such as superstructures formed with isostructural graphene, which are optimal to engineer gaps and doping, as well as to tune and enhance spin scattering.



However, this is easier said than done. Exploiting fine hBN-based nanostructures requires structural quality down to the atomic scale and precise lateral nano-structuration and integration with other two-dimensional materials, which lies beyond current lithographic capabilities. The bottom-up vapour growth is the alternative, which also works for 2D hybrids, although general procedures to control shape, size, and spatial order of surface phases are still lacking.



Lateral nanopatterning of hBN through epitaxial growth. The concept of the study of vicinal hBN/Rh interfaces is presented. CVD growth of hBN induces periodic (111)/(337) faceting of the Rh substrate. The hBN monolayer uniformly coats the faceted substrate, defining an effective lateral hBN/Rh heterointerface with periodic surface potential texturing. Using commercial Rh(111) films, one could exploit such chemical and electronic modulation of hBN to explore phonon–polariton THz excitations, selective growth of optically-active molecules, and vertical stacking with other 2D materials.

Hexagonal boron nitride nanostripes can be grown on vicinal rhodium surfaces

Now, a team of researchers from DIPC and other institutions has found a working disruptive approach: imprinting the lateral pattern of an atomically stepped one-dimensional template into a hBN monolayer. The researchers demonstrate the bottom-up synthesis of nanostriped hBN heterostructures with atomically sharp interfaces. The idea was to follow the standard chemical vapor deposition growth route, using rhodium (Rh) vicinal surfaces as one-dimensional (1D) templates. In practice, hBN was epitaxially grown on Rh surfaces using an Rh curved crystal for a systematic exploration, which produces a periodically textured, nanostriped hBN carpet that coats Rh(111)-oriented terraces and lattice-matched Rh(337) facets with tunable width.

Thus, a 1D lateral hBN (111)/(337) heterostructure arises, featuring defect-free boundaries and significant band offsets. The resulting electronic structure reveals a nanoscale periodic modulation of the hBN atomic potential that leads to an effective lateral semiconductor multi-stripe.

Since size tunability of phases can be gained by selecting the Rh vicinal plane, a variety of new possibilities are opened by this discovery. For example, the hBN (111)/(337) faceted system could be used as a model platform to mould and probe 1D phonon–polariton excitations in the THz regime, to achieve selective growth of atoms, aggregates, and molecular adsorbates for organic optoelectronics and catalysis, or to tailor the 3D stacking with other 2D materials, such as graphene.

DIPC HIGHLIGHT 2021

How aromatic are molecular nanorings? The case of a six-porphyrin nanoring

Casademont-Reig I, Guerrero-Avilés R, Ramos-Cordoba E, Torrent-Sucarrat M and Matito E
Angewandte Chemie International Edition 60, 24080 (2021)

Aromaticity is a property of cyclic structures with delocalized electrons, which give rise to some intriguing molecular properties: increased stability, certain geometrical features such as planarity, and exhibit a ring current under the presence of an external magnetic field. A molecule's aromatic character is typically verified experimentally using nuclear magnetic resonance (^{1}H-NMR), as the protons oriented toward the center of the ring are affected by the presence of the ring current in aromatic compounds.

Annulenes are monocyclic hydrocarbons that contain the maximum number of non-cumulated double bonds. They have the general formula C_nH_n (when n is an even number) or C_nH_{n+1} (when n is an odd number). Benzene is the smallest neutral annulene that presents π-conjugated aromaticity because it satisfies the Hückel rule, which states that molecules 4n+2 π electrons are aromatic. This rule helps to predict the aromaticity of relatively small annulenes, but it breaks for large annulenes. It is well established that large annulenes suffer out-of-plane distortions and exhibit a poor overlap between π orbitals, thus favoring non-symmetric conformations that are much less aromatic. The larger the annulene, the less aromatic the molecule is expected. For this reason, it is difficult to find large aromatic macrocycles. Geometrical constraints are actually imposed in some large macrocyclic structures with the hope of preserving conjugation, aromaticity, and quantum coherence.

Anderson and co-workers have recently synthesized and analyzed the aromaticity of a six-porphyrin nanoring (c-P6•T6) in four different oxidation states (c-P6•T6, c-P6T6^{4+}, c-P6•T6^{6}+, and c-P6•T6^{12+}), concluding from ^{1}H-NMR and computational analyses that c-P6•T6 and the c-P6•T6^{12+} are nonaromatic, whereas c-P6•T6^{4}+ and c-P6•T6^{6}+ are, respectively, antiaromatic and aromatic. c-P6•T6^{6}+ is thus one of the largest aromatic rings ever synthesized.

A team of researchers from DIPC demonstrates that the aromaticity of these large macrocycles is questionable. They provide compelling evidence that the conclusions are highly sensitive to the simulation employed, which should avoid the so-called delocalization errors. Using density functional approximations that minimize the delocalization error, they find that the main reason behind the absence of an aromatic ring current in these nanorings is the low delocalization in the transition from the porphyrins to the bridging butadiyne linkers, which disrupts the overall conjugated circuit. They also demonstrate that ^{1}H-NMR are not infallible probes of aromaticity and, therefore, the ^{1}H-NMR experimental evidence should not be blindly trusted.

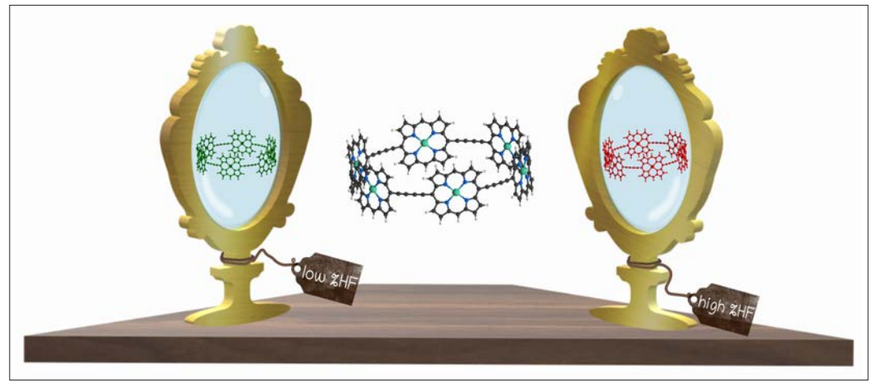
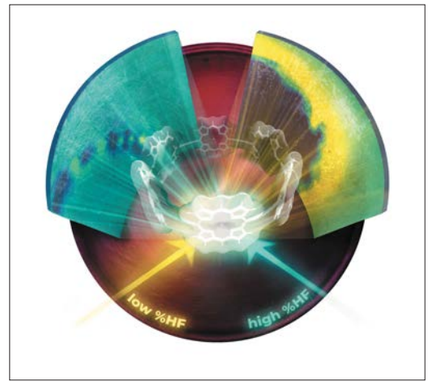


Figure 1. Methods with a low percentage of Hartree-Fock exchange suffer from delocalization errors and wrongly reflect the aromaticity of the nanoring structure.



Density functional approximations can suffer from delocalization errors that artificially increase the aromaticity of the molecule

Figure 2. Methods with a low percentage of Hartree-Fock exchange give a spuriously enhanced chemical shielding that suggests the presence of a ring current.

None of the large nanorings can be considered aromatic, and the quest for large aromatic nanorings should be continued. These results highlight the importance of choosing a suitable computational method to study large conjugated molecules and the appropriate aromaticity descriptors to identify the part responsible for the loss of aromaticity.

DIPC HIGHLIGHT 2021

Metallic carbon nanotube quantum dots with broken symmetries as a platform for tunable terahertz detection

Buchs G, Marganska M, González JW, Eimre K, Pignedoli CA, Passerone D, Ayuela A, Gröning O and Bercioux D
Applied Physics Reviews 8, 021406 (2021)

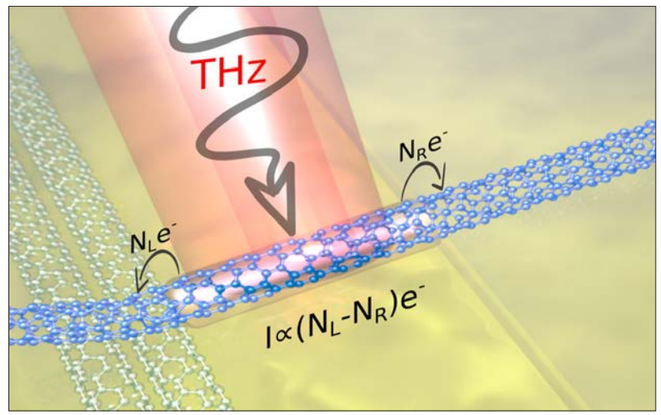
Terahertz (THz) radiation is all around us. For example, this page emits blackbody radiation mainly in the THz region (broadly from 0.3 THz to 30 THz). Because terahertz radiation begins at a wavelength of around one millimeter and proceeds into shorter wavelengths, it is sometimes known as the submillimeter band, and its radiation as submillimeter waves, especially in astronomy.

This band of electromagnetic radiation can be regarded either as microwave radio waves or far-infrared. The technology for its generation and manipulation is in its infancy; that is why engineers talk about the THz gap (in this case, from 0.1 to 10 THz). One of the reasons is that THz radiation from traditional microwave sources is usually too weak to have any measurable impact on the properties of materials.

The situation drastically changed at the beginning of the 2000s, when the technique of optical rectification with phase matching in crystals lacking inversion symmetry such as lithium niobate was developed. This technological breakthrough enabled the development of table-top sources of single-cycle THz pulses with field strengths comparable to the intrinsic field strength in a wide range of strongly correlated materials. Consequently, it became possible to modify their intrinsic fields to engineer new dynamic states of materials.

In condensed matter physics and in general, THz radiation is an efficient tool to investigate a multitude of low-energy excitations existing in the THz region. Important examples are resonances of phonons and plasmons (collective lattice and electron vibrations, respectively), spins, intersubband transitions (subbands are electronic energy bands formed in quantum wells, in which the electrons are confined in two directions), excitons (bound electron-hole pairs), macro-molecular vibrations and molecular rotations.

THz radiation can penetrate most dielectric materials non-invasively, opening the way for numerous possible applications in the fields of medicine, security, chemical spectroscopy, and data transmission, notably in the framework of the future 6, G cellular network. This is why photodetection and emission in the THz regime have recently attracted much attention from fundamental and applied research communities.



Proposed device to be used as either a high-resolution gate-tunable terahertz sensor or a broadband terahertz detector.

The proposed device is largely unaffected by temperatures up to 100 K, making carbon nanotube quantum dots with broken symmetries a promising platform to design tunable THz detectors that could operate at liquid nitrogen temperatures

A team of researchers, including the theorists from DIPC – Dario Bercioux & Andrés Ayuela – have proposed a theoretical scheme for a fully tunable THz detector based on carbon nanotubes. Specifically, using numerical simulations and scanning tunnelling spectroscopy, Buch et al. show that breaking simultaneously various symmetries in metallic nanotube quantum dots of arbitrary chirality strongly relaxes the selection rules in the electric dipole approximation removes energy degeneracies. This leads to a richer set of allowed optical transitions spanning frequencies from 1THz to several tens of THz for a ~10nm quantum dot. The researcher team proposed a terahertz detector device based on a metallic single-walled carbon nanotube quantum dot defined by artificial defects based on these findings. The operating regimes range from a high-resolution gate-tunable THz sensor to a broadband THz detector, depending on its length and contacts transparency. Their calculations indicate that the device is mainly unaffected by temperatures up to 100K, making carbon nanotube quantum dots with broken symmetries a promising platform to design tunable terahertz detectors that could operate at liquid nitrogen temperatures.

DIPC HIGHLIGHT 2021

A dissolution model of alite coupling surface topography and ions transport under different hydrodynamics conditions at microscale

Chen J, Martin P, Xu Z, Manzano H, Dolado JS and Ye G
Cement and Concrete Research 142, 106377 (2021)

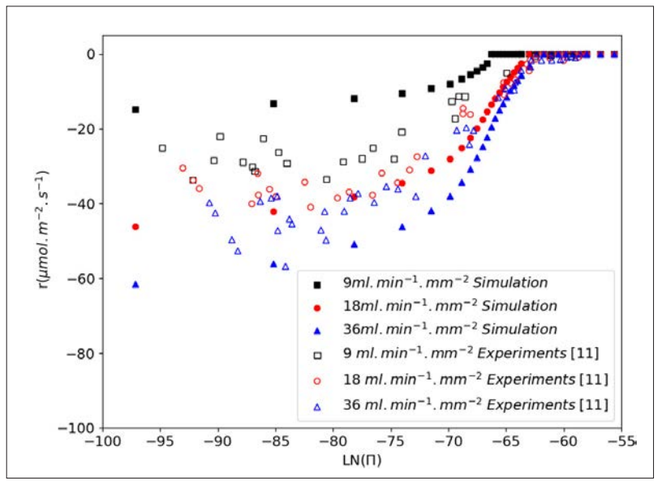
A cement is any of various substances used for bonding or setting to a hard material. A popular one, Portland cement, is a mixture of calcium silicates and aluminates made by heating limestone ($CaCO_3$) with clay (that contains aluminosilicates) in a kiln. The product is then ground to a fine powder. When Portland cement is mixed with water, it sets in a few hours and then hardens over a longer period of time due to the formation of hydrated aluminates and silicates.

Portland cement contains four main components: Alite, Belite, calcium aluminate and calcium aluminoferrite. Alite (tricalcium silicate) is the major and characteristic mineral phase. The thermodynamics and kinetics of Alite hydration has being studied for more than 100 years, still, it is not completely understood.

In the past decades, many hydration models were proposed for the hydration process of Portland cement. These models favored either particle reaction kinetics or integrated reaction kinetics, and focused on the dissolution of cement grains, but individual chemical components were not considered explicitly.

Some models have been proposed in order to predict the dissolution of alite. Some take the vector approach, with arbitrarily chosen hydration kinetics to calculate the hydration rate and convert the amount of hydration product into a volumetric term; however, thermodynamics and ions transport are not taken into account. Others proposed an analytical model to simulate the dissolution of alite. This model described the etch pit formation on the surface of Alite, and calculated the corresponding dissolution rate, but diffusion and chemistry were not considered.

In 2109, Pablo Martin, Hegoi Manzano and Jorge S. Dolado [Pablo Martin, Hegoi Manzano and Jorge S. Dolado (2019); *Advanced Theory and Simulations* doi: 10.1002/adts.201900114] proposed a Kinetic Monte Carlo model (KMC) at the nanoscale, which could simulate the dissolution of crystals not only in dilute solutions but also at close-to-saturated conditions. It simulated all dissolution mechanisms at nano/micro scales. Now, an integrated model is proposed to simulate the dissolution of Alite under different hydrodynamic conditions at microscale, combining KMC with the Lattice Boltzmann method (LBM) and the concept of diffusion boundary layer (DBL).



Influence of the flow rate on the dissolution rate of Alite for solutions having different initial calcium hydroxide concentrations. Comparison between the model and available experiments.

A integrated dissolution model is proposed to deal with different hydrodynamics conditions, coupling surface topography and ions transport

All aspects of the dissolution process are incorporated in the new model. The dissolution of Alite itself is modelled with KMC; two multiple-relaxation-time LBM models are used, one to simulate the flow and the other for the transport of ions. The solid-liquid interface is considered using an adapted DBL to calculate the concentration gradient and the dissolution flux. The model is validated with experimental data from literature.

The simulation results show good agreements with published results. At higher initial concentration, the simulation shows a greater dissolution rate than the experimental data. The plateau value is reached at saturated condition, which indicates that the simulation model can be used to predict the dissolution rate of Alite under extreme hydrodynamic conditions, i.e., high flow rates.

For a complete study on the dissolution of cement particle, it is necessary to involve all of its components individually and simultaneously. This new model for Alite provides a good start point for the simulation of the other cement components.

DIPC HIGHLIGHT 2021

Synthetic conjugates of ursodeoxycholic acid inhibit cystogenesis in experimental models of polycystic liver disease

Caballero-Camino FJ, Rivilla I, Herraez E, Briz O, Santos-Laso A, Izquierdo-Sanchez L, Lee-Law PY, Rodrigues PM, Munoz-Garrido P, Jin S, Peixoto E, Richard E, Gradilone SA Perugorria MJ, Esteller M, Bujanda L, Marin JJG, Banales JM and Cossío FP
Hepatology 73, 186 (2021)

Polycystic liver diseases (PLDs) are genetic disorders characterized by progressive development of symptomatic biliary cysts. Current surgical and pharmacological approaches are ineffective, and liver transplantation represents the only curative option. Ursodeoxycholic acid (UDCA) and histone deacetylase 6 inhibitors (HDAC6is) have arisen as promising therapeutic strategies, but with partial benefits. Here, we tested an approach based on the design, synthesis, and validation of a family of UDCA synthetic conjugates with selective HDAC6i capacity (UDCA-HDAC6i). According to our results, these UDCA-HDAC6i conjugates open a therapeutic avenue for PLDs.

Epigenetic enzymes have emerged as very promising therapeutic targets in medicinal and biological sciences. PLDs do not have any pharmacologically efficient treatment and constitute a heterogeneous group of genetic disorders characterized by progressive development of multiple fluid-filled biliary cysts (>10), which are the main cause of morbidity. Within this context, based on previous biological results, we decided to combine the structural and electronic features of UDCA with a spacer and a Zn-binding chelating group to generate by chemical synthesis a new family of conjugates able to inhibit histone deacetylases, especially cytoplasmic HDAC6.

Our chemical synthesis of the UDCA-HDAC6i molecules started with the coupling reaction of UDCA with amines to yield amide esters. Cleavage of the ester groups and in situ reaction with hydroxylamine or ortho-phenylendiamine permitted the isolation and characterization of UDCA-hydroxamates and ortho-aminophenylenamides shown in Figure 1 (a).

The potential HDAC6 inhibitory capacity of this family of UDCA synthetic conjugates was first evaluated in silico with a docking model (Figure 1 (b)). Significant binding affinities to HDAC6 were predicted for some of these compounds. Interestingly, three compounds oriented the hydrocarbon skeleton of UDCA toward the same region of the protein surface. We decomposed the total binding energy of each synthetic derivative into the contribution of different descriptors (i.e., hydrogen bonds, van der Waals and Coulombic interactions) to the overall score. Importantly, the contribution of UDCA to the final binding energy of UDCA-HDAC6i #1, #2, and #9 was approximately one-third of the total value, and was mainly integrated by van der Waals interactions and hydrogen bonds established by the two hydroxyl groups of the steroid skeleton of the BA.

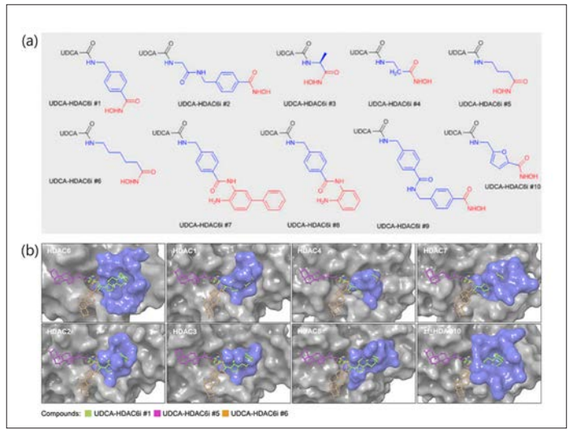
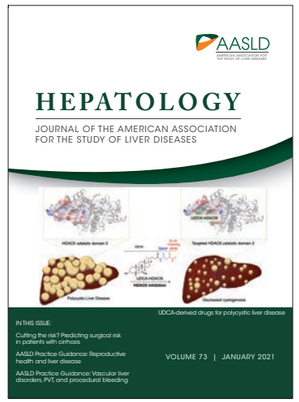


Figure 1. (a) Chemical structures of the UDCA-HDACi conjugates designed and synthetized for testing in animal models of polycystic liver diseases. (b) Optimized poses in docking experiments on human HDAC enzymes.

This novel family of histone deacetylase inhibitors opens a therapeutic avenue for polycystic diseases and other pathologies in which these enzymes play a significant role



Cover of Hepatology highlighting the therapeutic potential of our UDCA-HDACis.

This family of novel HDAC6is was tested in different biological assays and it was concluded that UDCA-HDAC6i #1 inhibited hepatorenal cystogenesis in vivo, improved ciliogenesis in cystic cholangiocytes, and inhibited their hyperproliferation. These therapeutic effects are superior to the simple sum of the individual or combined effects of its constituting pharmacologically active elements. These UDCA synthetic conjugates have preferential targeting to the liver through specific bile acid and organic cation transport properties and are highly concentrated into the enterohepatic circulation. These particular features make UDCA-HDAC6i molecules especially promising for the treatment of hepatic and gastrointestinal disorders where HDAC6 inhibition is considered a therapeutic target, such as acute liver failure, hepatocellular carcinoma, cholangiocarcinoma, pancreatic cancer, or colon cancer, among others, highlighting the high degree of translational potential of this family of chemical entities.

DIPC HIGHLIGHT 2021

Sensitivity of a tonne-scale NEXT detector for neutrinoless double-beta decay searches

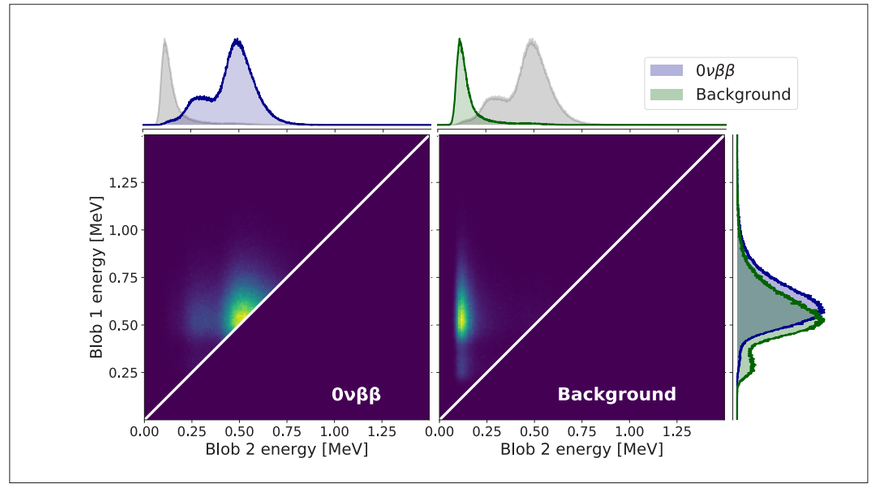
The NEXT collaboration, Adams C et al
Journal of High Energy Physics 8, 164 (2021)

NEXT-HD will optimize the ability to separate signal from backgrounds in terms of a topological signature. Thus its name, HD which refers to the high definition of the topological signature. In addition, NEXT-HD will deploy an excellent energy resolution (around 0.5 % FWHM at the relevant of the decay) and a very low radioactive budget. The combination of all these features, together with its large mass will increase the sensitivity to bb0nu processes by at least one order of magnitude with respect to NEXT-100, resulting in a large discovery potential.

The NEXT international collaboration formed and led by Ikerbasque Professor Gomez-Cadenas JJ, is developing the technology of High-Pressure Xenon gas Time Projection Chambers (HPXe) to search for neutrinoless double beta decay processes (bb0nu) in xenon. The detection of such events, in which an atom of the isotope Xe-137 decays into Ba-137, emitting two electrons and no neutrinos, would signal that the neutrino is its own antiparticle, a major discovery, which could explain, in particular, the cosmic asymmetry between matter and antimatter.

The NEXT collaboration is developing the HPXe technology in incremental steps. The initial prototype, NEXT-DEMO, with 1 kg of xenon, was followed by the successful NEXT-White demonstrator (10 kg of xenon), which has demonstrated the powerful topological signature (discussed below) low radioactive budget and excellent energy resolution of the technology. The NEXT-100 detector, deploying 100 kg of xenon is currently being commissioned at the Canfranc Underground Laboratory. NEXT-100 will reach a sensitivity to bbonu processes competitive with the best experiments currently in operation. In particular the experiment can make a discovery if the lifetime of the process is up to 1026 years.

Current data from oscillation experiments, however, suggest that the lifetime of bb0nu processes may be one order of magnitude larger (1027 years). If NEXT-100 does not find a signal, the next step is to build a detector with ten times more mass, while keeping the backgrounds from radioactive and cosmological events to essentially negligible levels.



The NEXT detectors are able to reconstruct the trajectory of the electrons moving in the chamber, measuring the energy of the end-points of the track. The signal (left) is characterized by high energy deposition in both end of the track (corresponding to two electrons), while the background only deposit energy in one of the ends. As shown in the figure, this allows a very effective separation between both types of events.

NEXT-HD will deploy an excellent energy resolution (around 0.5 % FWHM at the relevant of the decay) and a very low radioactive budget

The selected paper describes the main features and expected performance of such a detector, call NEXT-HD, which is currently being planned, and could start operations in about 5 years. Central to the large discovery potential of the NEXT detectors is their ability to discriminate the signal produced by bb0nu events (two electrons) from the spurious events produced by backgrounds, which result in single electrons, as illustrated in the figure.

Chemical tuning of exciton versus charge-transfer excited states in conformationally restricted arylene cages

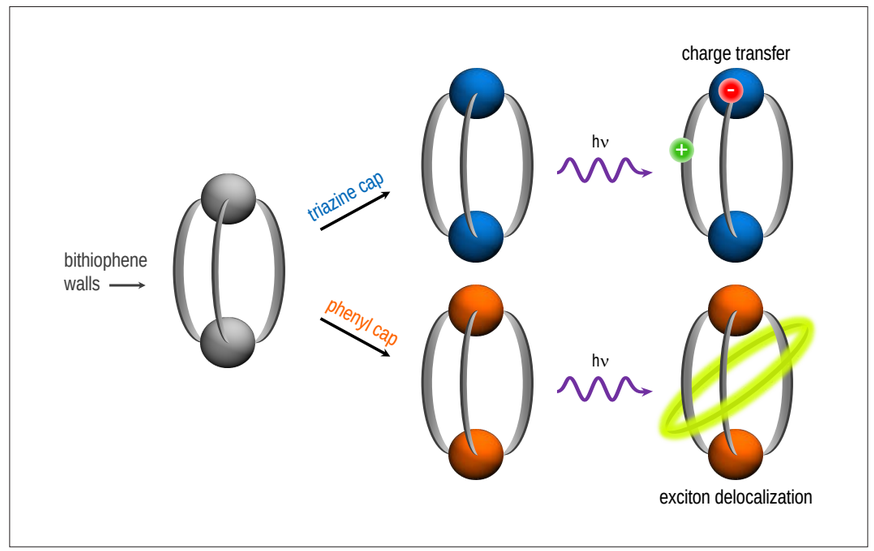
Lewis TN, Tonnelé C, Shuler WG, Kasun ZA, Sato H, Berges AJ, Rodriguez JR, Krische MJ, Casanova D and Bardeen CJ
Journal of the American Chemical Society 143, 18548 (2021)

Materials design for organic electronics requires to go beyond the molecular properties and address the solid-state properties instead, i.e., the collective behavior of multiple units in active layer thin films that depends on the supramolecular arrangement and nature of the intermolecular interactions. One major challenge thus lies in understanding and controlling these interactions, which can give rise to new emergent properties of the assembly.

Bulk solid-state samples, where disorder and the large number of interacting molecules make difficult a first-principles description, are not the best place to start. This complexity motivated the synthesis and study of discrete multiunit assemblies of conjugated molecules with controlled chemical and geometrical structures and restricted conformational freedom that can be purified and studied in isolation, for example, in dilute solution. Examples of such conjugated assemblies include donor-bridge-acceptor molecules, bichromophores and dendrimers. In these supermolecules, covalent linker groups define both the number and connectivity of the interacting conjugated subunits.

Yet, even in these smaller systems, the conformational flexibility of covalent assemblies can lead to multiple configurations that have different subunit interactions and, consequently, different electronic states and dynamics. In many cases, the conformational freedom of these covalent assemblies complicates their interpretation as structurally well-defined model systems. Additionally, although we would like to assume that the linker is inert, the truth is that a large body of work says otherwise, showing that it can play an important role in facilitating charge and energy transfer. Any new architecture that would limit conformational freedom and help establish the actual role of the linker would be, thus, most welcome.

In a combined theoretical/experimental study, a team of researchers used a novel cage architecture to demonstrate how chemical tuning can allow to precisely control the nature of the excited states. In particular, they reported the synthesis and photophysics of two triple-stranded thiophene based cages differing in the nature of the aromatic cap, namely benzene and triazine, that links the individual branches of the cage at both top and bottom. This strategy enables improved control of both molecular spacing and orientation as it provides two points of attachment for each conjugated subunit, bringing the assembly closer to crystalline order. Furthermore, the capping group acts as a constant structural element while providing chemical tunability that can be used to actively modify the electronic structure of the assembly.



Schematic of capped bithiophene cage. Dependent on the capping unit used to lock the bithiophenes into the cage conformation, it can undergo charge transfer or exciton delocalization.

Chemical tuning of novel multichromophoric cage architecture enables engineering of excited states nature

Combining steady-state and time-resolved spectroscopies and (time-dependent) density functional theory calculations, they showed that an inert benzene cap supports through-space interchromophore Coulomb interaction generating a neutral Frenkel H-type exciton state that can undergo rapid intersystem crossing (ISC), in turn associated with a strongly decreased fluorescence. On the contrary, using a triazine cap allows the formation of low-lying charge transfer states that can avoid ISC and enhance the fluorescence quantum yield.

The ability to create different nanoscale heterostructures while retaining the overall morphology provides an unprecedented opportunity to tune the properties of these discrete assemblies. These results provide a new route toward structurally well-defined multichromophoric assemblies whose excited states can be rationally designed using the tools of organic synthesis and computational chemistry. As this architecture is in principle scalable, it may provide a path to systematically bridge the gap between molecular properties and solid-state material performance.

DIPC HIGHLIGHT 2021

The BACCO simulation project: exploiting the full power of large-scale structure for cosmology

Angulo RE, Zennaro M, Contreras S, Aricò G, Pellejero-Ibañez M and Stücker J
Monthly Notices of the Astronomical Society, 507, 5869 (2021)

This paper presents a new suite of supercomputer simulations of the nonlinear gravitational interactions of matter in the Universe. These calculations were then used to train artificial intelligence algorithms to generate millions of new synthetic universes. These predictions will be used to interpret observations made by the forthcoming ESA's satellite mission "Euclid".

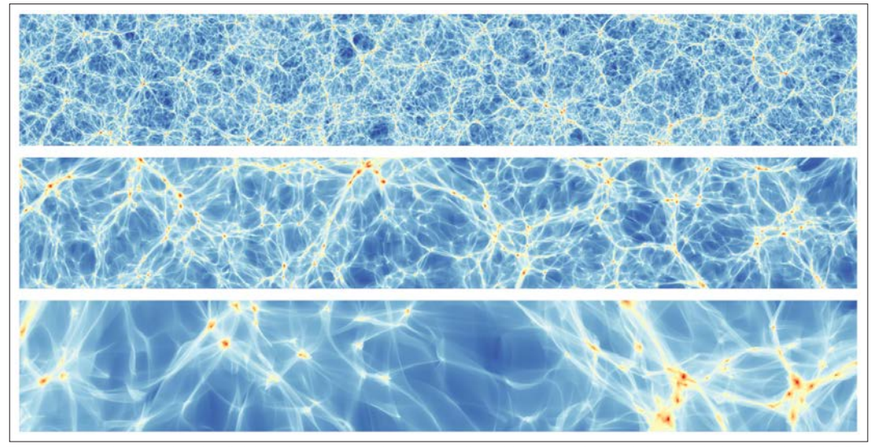
Over the last 20 years, our understanding of the Universe has grown tremendously. There is a relatively simple model, referred to as LCDM, which can explain the main observed properties of the Universe – from its infancy state to the present-day structure. There are, however, major unanswered questions in this model. For instance: the nature of dark energy that causes an accelerated cosmic expansion, the origin of the seeds from which structure emerged, and the properties of "dark matter" – the most abundant form of mass in the Universe.

In the upcoming years, a new generation of telescopes – located in different places around the world and in outer space – will map the distribution of dark matter, gas, and millions of galaxies. This will offer the possibility of profound discovery. We will be able to carry out tests where perhaps Einstein's General Relativity will break down, a new fundamental particle will appear, or where we would find a clue to explain the accelerated cosmic expansion.

The goal of this paper is to increase the chances for such discoveries by developing a new generation of supercomputer simulations mimicking large regions of the Universe. These simulations – designed to match the new telescopes' observations – have generated hundreds of virtual universes which can be compared to the real one. In each of these computer-generated universes, various cosmic ingredients are varied: the strength of gravity; the processes that govern the formation of galaxies; and the amount of massive neutrinos, dark matter, spatial curvature.

Cosmological simulations typically need tens of thousands of computer cores and millions of hours in computing time, thus it is only possible to carry them out for a small number of parameter sets. To avoid this limitation, we have used existing simulations to train neural networks which are able to create new predictions in unseen parameter sets in under one second of computer time. This enables a thorough exploration of the cosmological parameter space, finding the combination that best describes the observed Universe.

Supercomputer simulations are needed to understand the nonlinear processes that give rise to complexity in the universe



The projected mass density field at the present day, as predicted by one of the eight simulations in the BACCO suite. Each image corresponds to a 100 million light-years deep projection employing a phase-space interpolation method. Top, middle, and bottom panels progressively zoom onto regions 6, 1, and 0.4 billion light-years across.

These tools are currently being incorporated in the data analysis pipeline of the "Euclid" mission. "Euclid" is a satellite telescope developed by the European Space Agency with an expected launch in February 2023. Euclid will detect around 10 billion astronomical sources with which it will map the distribution and evolution of dark matter in over a third of the sky. This will be the most detailed map of the cosmos ever made.

By combining Euclid's data with supercomputer simulations and machine learning, it will be possible to find signatures that distinguish between competing theories for, e.g., dark matter or for the origin of the Universe. We will also be able to investigate whether we can explain the distribution of galaxies and matter within our current galaxy and structure formation theories and whether it will be necessary to include new ingredients, or even change the laws of physics!

DIPC HIGHLIGHT 2021

Van der Waals driven anharmonic melting of the 3D charge density wave in VSe_2

Diego J, Said AH, Mahatha SK, Bianco R, Monacelli L, Calandra M, Mauri F, Rossnagel K, Errea I and Blanco-Canosa S

Nature Communications 12, 598 (2021)

A charge density wave (CDW) is a many-body state of matter characterized by the static modulation of conduction electron density together with the corresponding crystal lattice distortion. Phase transitions to this electronic charge ordering state have been reported in many low dimensional materials at low temperatures, in which there is a big debate on the interplay with the superconducting phase. Indeed, the origin and stabilization of this phenomenon is still an underdebate topic, especially in high dimension systems, as it is the case of quasi-2D layered transition metal dichalcogenides (TMDs). TMDs are particularly interesting because they are the first crystalline structures where 3D CDWs were discovered. Their high dimensionality may imply that the one-dimensional Fermi surface nesting scenario may not be entirely suitable, acquiring electron-phonon interaction particular importance.

The CDW transition of some TMD compounds like 2H-$NbSe_2$ and 1T-$TiSe_2$ has been found to be characterized by the softening of a low energy acoustic phonon branch at the critical wave vector, which goes to zero frequency at the transition temperature. In this work we study this behaviour both experimental and theoretically in the 1T phase of VSe_2, which develops a complex 3D incommensurate pattern in its CDW phase with a q_{CDW} = (0.25 0 –0.3) r.l.u CDW wave vector. Motivated by the good results obtained, we finally analyze the origin of the CDW in VSe_2.

This work is the result of a cooperative work between experimentalists and theoreticians. Our high-resolution inelastic x-ray scattering experiments have shown for the first time that the CDW transition in this compound is characterized by the collapse at 110K of a low energy acoustic mode. This behavior has been ratified by our ab initio anharmonic phonon calculations with the stochastic self-consistent harmonic approximation (SSCHA), a variational method that fully accounts for non-perturbative anharmonic effects. These theoretical calculations have pointed to anharmonicity as the responsible for stabilizing the 1T phase of VSe_2 at high temperatures. Indeed, remarkably our theoretical phonons are only comparable to experimental results if interlayer weak van der Waals corrections are considered. Definitely, both anharmonic effects and van der Waals interactions between neighbouring VSe_2 layers are vital to melt the CDW.

The dominant role of van der Waals forces here may be attributed to the out-of-plane nature of the CDW, which modulates the interlayer distance. This is not the case in 2H-$NbSe_2$, where the bulk and monolayer transition temperatures seem to be similar as reported experimentally by Ugeda et al. and theoretically by Bianco et al. This line of thinking is consistent with the enhancement of the CDW in monolayer VSe_2, since the out-of-plane van der Waals interactions are absent in this case.

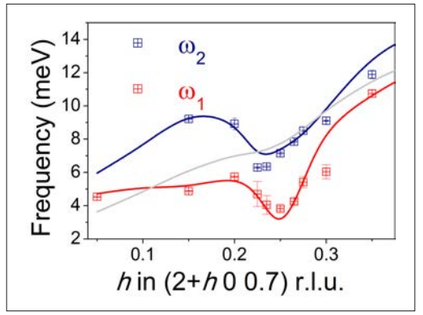


Figure 1. Momentum dependence of the frequency of the ω_1 and ω_2 branches at 150 K. The anharmonic phonon dispersions of the acoustic modes obtained at 150 K are plotted as solid lines. The gray line represents the acoustic mode that is silent in IXS.

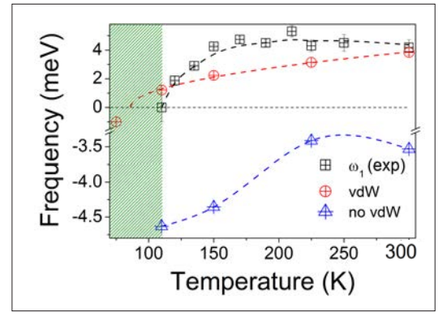


Figure 2. Temperature dependence of the energy of the ω1 CDW driving branch and the anharmonic theoretical frequencies obtained with and without van der Waals corrections. The shaded area defines the CDW region.

Definitely, both anharmonic effects and van der Waals interactions between neighbouring VSe_2 layers are vital to melt the CDW

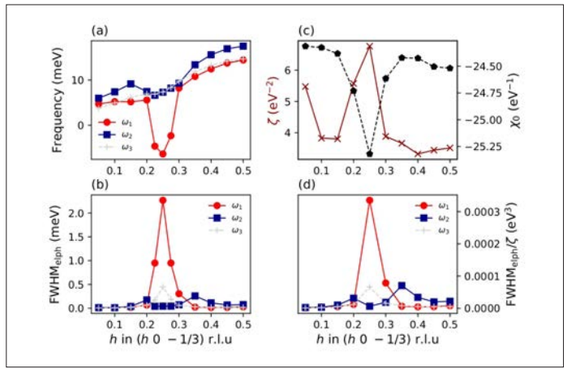


Figure 3. Electron–phonon interaction vs Fermi surface nesting. (a) Calculated harmonic phonon spectra of 1T-VSe_2 along (h 0 -1/3) r.l.u. Only acoustic modes are shown. The gray line denotes the mode silent in IXS, which is labeled as ω3 here. (b) Phonon linewidth (full width at half maximum) given by the electron–phonon interaction for the same modes. (c) Real part of the non-interacting susceptibility, χ_0, as well as the nesting function, ζ, at the same wave vectors. (d) Ratio between the full width at half maximum given by the electron–phonon interaction and the nesting function.

Finally, our work sheds light on the crucial role of the EPI and nesting mechanism in the formation of the charge modulated state. We conclude that the electron-phonon interaction is the main driving force of the CDW transition in 1T-VSe_2 despite the presence of nesting at the critical wave vector. This conclusion is supported by the wide softening in momentum space observed in the experiments, in addition to the calculated strongly momentum dependent electron–phonon linewidth peaking at the critical wave vector, and the weaker dependence on the wave vector of the susceptibility.

DIPC HIGHLIGHT 2021

Complex plasmon-exciton dynamics revealed through quantum dot light emission in a nanocavity

Gupta SN, Bitton O, Neuman T, Esteban R, Chuntonov L, Aizpurua J and Haran G
Nature Communications 12, 1310 (2021)

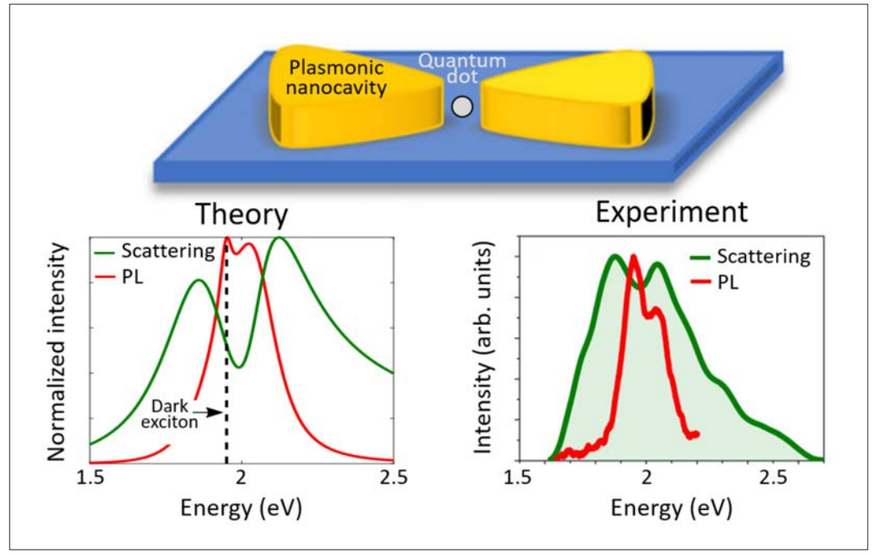
Light emitted by quantum dots coupled to plasmonic nanocavities and the underlaying dynamics of the excited states in the system can be strongly affected by dark excitonic states in the quantum dots, as recently revealed by a combined theory-experiment study of the system scattering spectrum, photoluminescence and two photon correlations.

The manipulation of optical transitions in semiconductor materials enables new possibilities to engineer the absorption and emission of light, with applications such as the design of more energetically efficient light sources. For example, discrete atom-like excitonic states at optical energies are obtained by fabricating structures of nanometric size in all three dimensions, so-called quantum dots.

The properties of quantum dot excitonic states are not intrinsic, but can be modified by the surrounding environment. A particularly large modification of the optical properties of quantum dots can be produced when interacting with metallic nanocavities (sketch in top panel of the figure). These nanocavities present plasmonic resonances produced by collective oscillations of the free electrons in the metal, and are able to localize electromagnetic energy into very small volumes, leading to very efficient coupling with excitons. A typical effect of plasmons is to induce an increase of the exciton radiative rate, of interest in the design of fast and efficient light sources. For very intense exciton-plasmon interaction, the regime of strong coupling is achieved, characterized by the emergence of new polaritonic modes that combine the properties of the excitons and those of the plasmonic resonances.

The study of emission dynamics in quantum dots usually focuses on bright excitonic states that radiate photons efficiently and can be easily excited by a laser, while difficult-to-excite dark excitons are often ignored. In this work, DIPC researchers use a cavity electrodynamics framework to show that a dark excitonic state in a quantum dot can play a key role in the dynamics of a coupled plasmonic cavity-quantum dot system, which allows for explaining several unexpected experimental findings by colleagues at the Weizmann Institute of Science in Israel (bottom panels in the figure). The dark exciton does not significantly affect the light scattered or absorbed at the energy of the illumination laser, but it does strongly modify the photoluminescence spectrum as well as the behaviour of the two-photon correlations, a key property to identify the emission of non-classical light. These results thus emphasize the importance of considering both bright and dark excitons to fully understand the optical response of complex nanoscale systems formed by plasmonic nanostructures coupled to one or a few quantum dots.

Light emission of quantum dots in plasmonic antennas reveals a complex excitonic dynamics



Coupling of a quantum dot and a plasmonic nanocavity. Top: sketch of the system considered, where a quantum dot interacts with a plasmonic nanocavity. In the experimental realization a bowtie configuration is used with two triangular nanoparticles separated by a very narrow nanogap. The system is close to the strong coupling regime. Bottom left: calculated scattering spectra (light emitted elastically at the frequency of the illumination) and photoluminescence, PL, spectra (light emitted inelastically at lower energy than the illumination). Bottom right: measured scattering and PL spectra. In both theory and experiments the spectral shape of the scattering is very different to that of the PL, showing spectral peaks of different width and at different positions, attributed to the presence of a dark exciton in the quantum dot.

DIPC HIGHLIGHT 2021

Topological phase transition in chiral graphene nanoribbons: from edge bands to end states

Li J, Sanz S, Merino-Díez N, Vilas-Varela M, Garcia-Lekue A, Corso M,
G de Oteyza D, Frederiksen T, Peña D and Pascual JI
Nature Communications 12, 5538 (2021)

In the last decades, a mathematical description of symmetries in nature called topology has been applied to describe and predict new electronic and magnetic properties of materials. A very simple aspect of topology connects a symmetry in the atomic structure of a crystal with a class of materials. Many materials that we know or use in current technology (silicon, diamond, gallium arsenide, etc.) belong to a topological class called trivial, meaning standard, and behave as normal semiconductors or insulators.

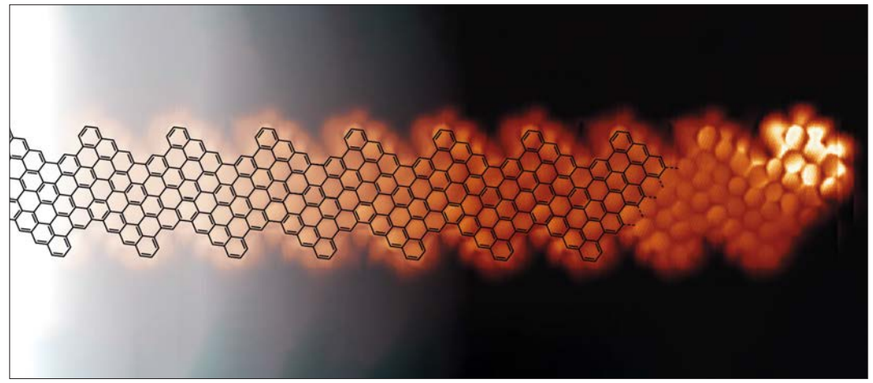
Novel materials with "anomalous" topology (technically called non-trivial) can be fabricated with advanced techniques of material science, which achieve control of their structure with atomic precision. For such materials, mathematical models predict "exotic" properties that can be utilized in future technology, such as that they are insulating inside and metallic at their surfaces.

In this study, published in Nature Communications a multidisciplinary group of Spanish research teams reported that certain stripes of graphene called graphene nanoribbons (GNRs) acquire the anomalous topological state of matter when narrowed down to just a few nanometres in width.

GNRs are atomically thin, planar carbon nanostructures that can be obtained from a sheet of graphene (carbon atoms arranged in a hexagonal lattice) by cutting in different directions. Conceptually, they can be thought of as stripes of graphene aligned along different directions, i.e., as nanoscale wires that may be used to transport an electronic current.

The scientists fabricated with atomic precision narrow GNRs of different width and orientation, like in the figure below, and demonstrated that all types convert from a metallic into an insulating state when the width is reduced below a few nanometers. Unexpectedly, they found that this new state corresponds to a non-trivial topological class.

Because of their anomalous topology, electronic states were found localized at the ends of the ribbons (as shown in the figure). These states represent a novel source of non-conventional magnetism with promising applications in quantum technologies.



Scanning tunneling microscopy image resolving the hexagonal structure (schematically indicated by black lines) of one of the studied GNRs. The bright, localized feature at the right side reveals the emergent "exotic" state at the end of the ribbon.

Novel electronic states were found at the end of specific chiral graphene nanoribbons

This study was achieved through a multidisciplinary collaboration combining tools and methods of chemistry and physics. First, organic chemists at the CIQUS institute in the University of Santiago de Compostela synthesized molecular precursors for GNRs using solution chemistry. Physicists at CIC nanoGUNE and at the Centro de Física de Materiales (CFM), in San Sebastian, did the assembling reaction on metal surfaces to produce the desired GNRs with atomic precision and investigated their anomalous electronic properties with scanning tunneling microscopy. The physicists at the Donostia International Physics Center (DIPC) did theoretical simulations that demonstrated the anomalous topology of the narrow GNRs. This result widens the scope for the use of graphene nanostructures in emerging quantum technologies

DIPC HIGHLIGHT 2021

Cubic 3D Chern photonic insulators with orientable large Chern vectors

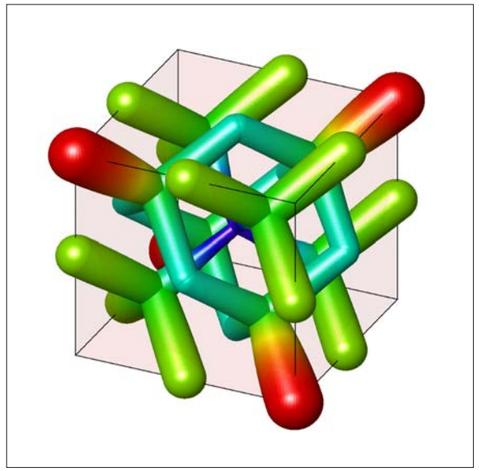
Devescovi C, García-Díez M, Robredo I, Blanco de Paz M, Lasa-Alonso J, Bradlyn B, Mañes JL, Vergniory MG and García-Etxarri A
Nature Communications 12, 7330 (2021)

Some materials have special universal properties protected against perturbations. Such properties are theoretically described by topology, a branch of mathematics concerned with the properties of geometrical objects that are unchanged by continuous deformations. So-called topological insulators are electronic materials that have a bulk band gap like an ordinary insulator but have conducting states on their boundaries, i.e., edges or surfaces. The conducting surface is not what makes topological insulators unique, but the fact that it is protected due to the combination of spin-orbit interactions and time-reversal symmetry.

A topological invariant is a geometrical quantity that remains unchanged by continuous deformations. Topological invariants have found widespread applications in physics, chemistry, and materials science. One of the best known topological invariants in condensed matter physics is the Chern number.

The definition of the Chern number is not exactly simple. But it could be enough to understand the Chern number as an integer that characterizes the topology of filled bands in two-dimensional lattice systems. A band with a non-zero Chern number is topologically non-trivial. When the highest occupied band is non-trivial and completely filled, the state is called a topological insulator. A material whose topological phases can be characterized by the Chern number is called a Chern insulator, a class of topological insulators.

But when we make Chern insulators interact with light, something interesting happens. Electrons are spin-1/2 particles, whereas photons are spin-1 particles. The distinct spin difference between these two kinds of particles means that their corresponding symmetry is fundamentally different. An electronic topological insulator is protected by the electron's spin-1/2 (fermionic) time-reversal symmetry; however, due to photon's spin-1 (bosonic) time-reversal symmetry, the same protection does not exist under normal circumstances for a photonic topological insulator. In other words, we could have a Chern photonic insulator with broken time-reversal symmetry. Time reversal symmetry broken topological phases provide gapless surface states protected by topology, regardless of additional internal symmetries, spin or valley degrees of freedom. Thus, the topology of the propagation of light in photonic crystals has been the subject of much recent attention.



Unit cell of on of the designed 3D Photonic Chern insulators.

Our team of researchers proposes a method to design cubic 3D topological photonic crystals where Chern vectors of any magnitude, sign or direction can be implemented at will

Despite the numerous demonstrations of 2D topological phases, few examples of 3D topological systems with time reversal symmetry breaking exist. In contrast to 2D, a 3D Chern insulator is a topological phase that can be characterized by three first Chern invariants–or a Chern vector C = (Cx, Cy, Cz) – defined on lower dimensional surfaces: such a state of matter can support chiral surface states propagating on the planes with Miller indices indicated by the Chern vector.

Now, our team of researchers proposes a method to design cubic 3D topological photonic crystals where Chern vectors of any magnitude, sign or direction can be implemented at will. The new method is based on the merging and annihilation of Weyl points through multifold supercell modulations in three dimensions. The designs achieved this way display topologically protected chiral and unidirectional surface states with disjoint equifrequency loops.

The resulting crystals present the following characteristics: First, by increasing the Chern number, multiple surface states channels can be supported. Second, the Chern vector can be oriented along any direction simply changing the magnetization axis, opening up larger cube/cube interfacing possibilities as compared to 2D. Third, by lowering the time reversal symmetry breaking requirements, the system is ideal for realistic photonic applications where the magnetic response is weak.

DIPC HIGHLIGHT 2021

Avoiding a replication crisis in deep-learning-based bioimage analysis

Laine RF, Arganda-Carreras I, Henriques R and Jacquemet G
Nature Methods 18, 1136 (2021)

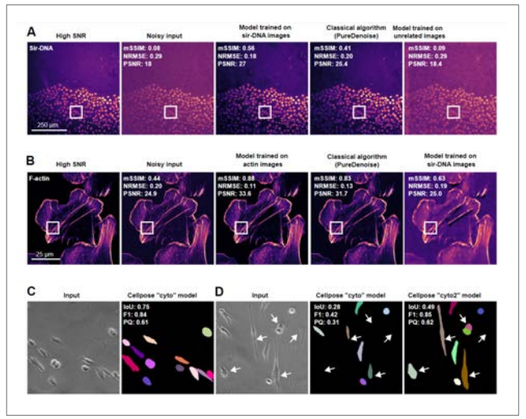
Microscopy is a leading technology in biological research. Today, a typical microscopy session may generate hundreds to thousands of images, generally requiring computational analysis to extract meaningful results. But a simple analysis is not enough any more. Over the last few years, deep learning (DL) has increasingly become one of the gold standards for high-performance microscopy image analysis. DL algorithms have become powerful tools for analyzing, restoring and transforming bioimaging data. One promise of DL is parameter-free one-click image analysis with expert-level performance in a fraction of the time previously required. Is it a realistic promise? As with most emerging technologies, the potential for inappropriate use is raising concerns among the research community, what should we do to make sure the results provided are reliable and reproducible?

For image analysis, DL usually uses algorithms called artificial neural networks (ANNs). Unlike classical algorithms, before an ANN is used, it first needs to be trained. During training, the ANN is presented with a range of data, from which it attempts to learn how to perform a specific task. More specifically, the ANN builds a model of the mathematical transformation that needs to be applied to data to obtain the desired output. ANNs can therefore be considered as non-linear transformation machines, performing sequential mathematical operations on the input data. As we inspect deeper into these sequences of operations, it becomes difficult to understand what features of the original images are used. For that reason, they are often thought of as 'black boxes' as, for most users, only the input images and output predictions are readily available.

Learning how to perform an analysis from example data is both the principal strength and the main weakness of DL. By learning directly from the data, the ANN tries to identify the most suitable way to perform the analysis, leading to models with excellent performances for that particular dataset. However, trained DL models are only as good as the data, and the parameters used to train them. Thus, one powerful approach is to produce general models with high reusability potential using a large and diverse training dataset.

As DL models are becoming accessible through public repositories (so-called model zoos, such as bioimage.io) or web interfaces, it becomes straightforward to use the models directly to analyze new data. This has the advantages of speeding up DL uptake but, unless the researchers can confirm that their own data were well-represented within the training dataset used initially (which can be very difficult to do), the performance of such portable models on the new data often remains unclear.

This is the reason why despite its incredible potential, the application of DL in microscopy analysis has raised concerns due to a lack of transparency and understanding of its limitations, especially for generalizability. In addition to this, DL is developing at an incredible rate, which places a significant burden on users to determine the most appropriate tools for their needs. It remains challenging to assess the validity and performance of a range of approaches that are often difficult to compare, especially when widely accepted benchmark datasets are unavailable.



Deep learning (DL) methods can offer excellent performances but only when the model used matches the data to be analysed. a,b, Noisy images of cells stained to visualize their nuclei (a) or F-actin (b) were acquired using a spinning disk confocal microscope and denoised using two different DL (CARE) models or a classic algorithm (PureDenoise). One DL model was trained to denoise these images, while the other was trained to denoise structured illumination microscopy images of F-actin. Note that in both cases, the appropriate DL model outperforms the classic algorithm, while the inappropriate DL model fails to denoise these images correctly. In b, the inappropriate DL model was trained to denoise the nuclei images shown in a. c,d, Examples to highlight how segmentation models can offer variable performance even on similar images. Images of cells migrating on cell-derived matrices were acquired using a brightfield microscope and segmented with DL models (cellpose). Note how the DL cyto model performs well in c but poorly in d. Also, note how the DL cyto2 model, a model trained with additional data, performs better than the cyto model in d.

Spiderman's Uncle Ben has never been more right than today: "With great powers comes great responsibility"

Now a team of researchers at Universidad del Pais Vasco, University College London, Instituto Gulbenkian de Ciência and Åbo Akademi University, in order to help define adequate guidelines and ensure the appropriate use of this transformative technology, has reviewed key concepts that they believe are important for researchers to consider when using DL for their microscopy studies. They also describe in this work how results obtained using DL can be validated and propose what should, in their view, be considered when choosing a suitable tool. Finally, they also suggest what aspects of a deep learning analysis should be reported in publications to ensure reproducibility.

The researchers argue the importance of validating any model using a purposefully built evaluation dataset containing ground-truth target images or labels. Similarly, the use of DL models should be reported appropriately to ensure reproducibility and transparency. This is a challenging task for DL as many components, both internal (hyperparameters) and external (training dataset) to the network used, can dramatically influence the results obtained.

With the increasing availability of networks and models, finding ways to identify what might be a 'good tool' becomes critical. The authors believe that a good tool should not be only a performant one, but that its transparency of what it does to the data, usability and reliability are equally important.

The responsibility of proper use of DL in microscopy is now equally shared between users and developers. Spiderman's Uncle Ben has never been more right than today: "With great powers comes great responsibility".

DIPC HIGHLIGHT 2021

Time for NanoNeuro

Garcia-Etxarri A and Yuste R
Nature Methods 18, 1287 (2021)

Because of their unique physical properties, nanomaterials have intrinsic advantages as biosensors and actuators, and they may be applicable to humans without the need for genetic modifications. It follows, then, that nanoscience could make major methodological contributions to the future of biomedical sciences, especially neuroscience. Meet NanoNeuro, a new field defined as the intersection of nanoscience and neuroscience, that aims to develop nanoscale methods to record and stimulate neuronal activity.

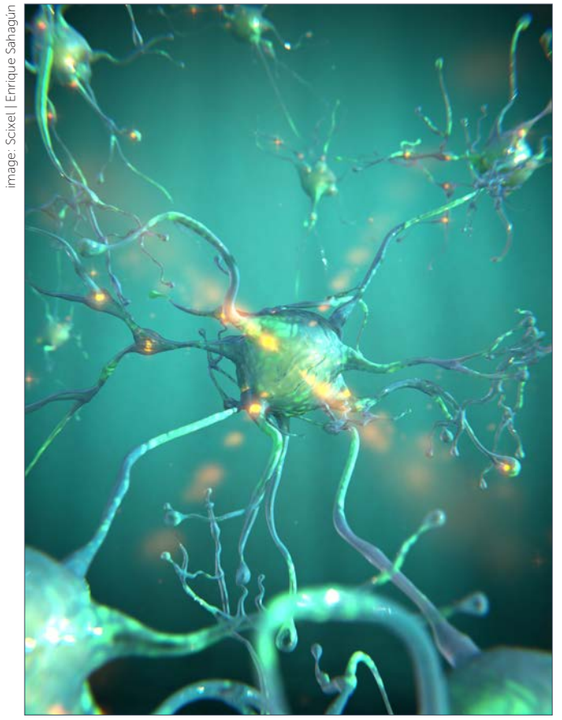
Traditional neuroscience tools, such a metal or glass-based electrodes, have been used for over a century to record the activity of individual neurons, but are inadequate for characterizing the function of vast numbers of them in their form in the brain. More recently, optical imaging using fluorescent calcium or voltage probes and magnetic resonance imaging, which detects haemoglobin oxygenation, have enabled a more comprehensive recording of neural circuits. Still, in terms of spatial and temporal resolution, current methods are far from recording 'every spike from every neuron'.

Methods for manipulating brain activity have similar shortcomings in spatio-temporal resolution. For example, traditional stimulating electrodes, used in the clinic for deep-brain stimulation, and newer optical and magnetic methods for activating single neurons or groups of them, either with optogenetics, optochemistry, or transmagnetic stimulation, are still far from achieving systematic stimulation of entire neural circuits, with single-cell precision, in three dimensions (3D) in awake, behaving animals. To perform such a systematic recording and manipulation of neural circuits, new technologies are necessary.

In 1959, Richard Feynman, in his talk 'There's Plenty of Room at the Bottom', described the possibility of chemical synthesis by direct manipulation of atoms, thus marking the start of nanoscience. Aside from being a technological breakthrough, nanomaterials have enabled the development of new technological tools and the discovery of new physical laws. Indeed, over the last few decades, nanomaterials with previously unknown properties and functions have been developed, with applications in research fields ranging from electronics and energy harvesting to biomedicine.

In order to learn where NanoNeuro currently stands, Aitzol Garcia-Etxarri and Rafael Yuste discuss in a review article nanoscience-based methods and tools to record and stimulate neuronal activity as a potential technological platform to propel neurotechnology forward. They consider both electrode and particle-based approaches to these methods.

image: Scixel | Enrique Sahagun



Artistic view of nanoparticles interacting with neurons to record and induce neural activity.

Nanoscience-based methods and tools to record and stimulate neuronal activity

The authors find that the NanoNeuro is still in its infancy as a scientific field. From the variety of approaches they discuss, it is clear that there is not a one-size-fits-all method, as different nanomaterials have different advantages and disadvantages when compared with existing neuroscience methods. They envision a future where the combination of nanomaterials with existing methods facilitates the creation of new and powerful hybrid technologies. But, there are substantial challenges that NanoNeuro methods should still overcome to reach technological maturity and to enable real-world applications.

Probably, one of the major challenges will be the isolationist tendencies of scientific fields. For NanoNeuro to grow, it will be necessary to break barriers betweeWn disciplines, with strong collaborations and interdisciplinary training for the next generations. Because, paraphrasing Feynman, there's plenty of room at the bottom, also for neuroscience.

DIPC HIGHLIGHT 2021

Real-space observation of vibrational strong coupling between propagating phonon polaritons and organic molecules

Bylinkin A, Schnell M, Autore M, Calavalle F, Li P, Taboada-Gutièrrez J, Liu S, H. Edgar J, Casanova F, Hueso Luis E, Alonso-Gonzalez P, Y Nikitin A and Hillenbrand R
Nature Photonics 15, 197 (2021)

Van der Waals materials consist of two-dimensional layers bound by weak van der Waals forces. After the isolation of graphene, the field of two-dimensional van der Waals materials has experienced an explosive growth and new families of two-dimensional systems and block-layered bulk materials have been created.

This growth has been fueled mainly by the possibility of tuning a set of remarkable electronic properties using a variety of methods (thickness control, doping, intercalation, proximity effects, to name a few) and a relative simplicity of fabrication. These two characteristics, that make layered van der Waals materials similar to Lego constructions, are attractive from both practical and fundamental points of view.

In a parallel development, phonon polaritons — the result from the coupling of an infrared photon with an optic phonon — with extraordinary properties have been discovered in polar van der Waals crystals. A remarkable example is a dielectric hexagonal boron nitride (h-BN), where such exotic phenomena as ray propagation or hyper-lensing effects can be observed, offering opportunities for the development of a planar directional control of light–matter interactions at the nanoscale.

Since phonon polaritons in h-BN spectrally coincide with typical mid-infrared molecular vibrational resonances, these polaritons could be a way to achieve a strong vibrational coupling. Theoretically, this interaction could be the key for developing ultrasensitive infrared spectroscopy and a new way to modifying chemical properties of molecules. However, until now this most interesting interaction has not been proven experimentally.

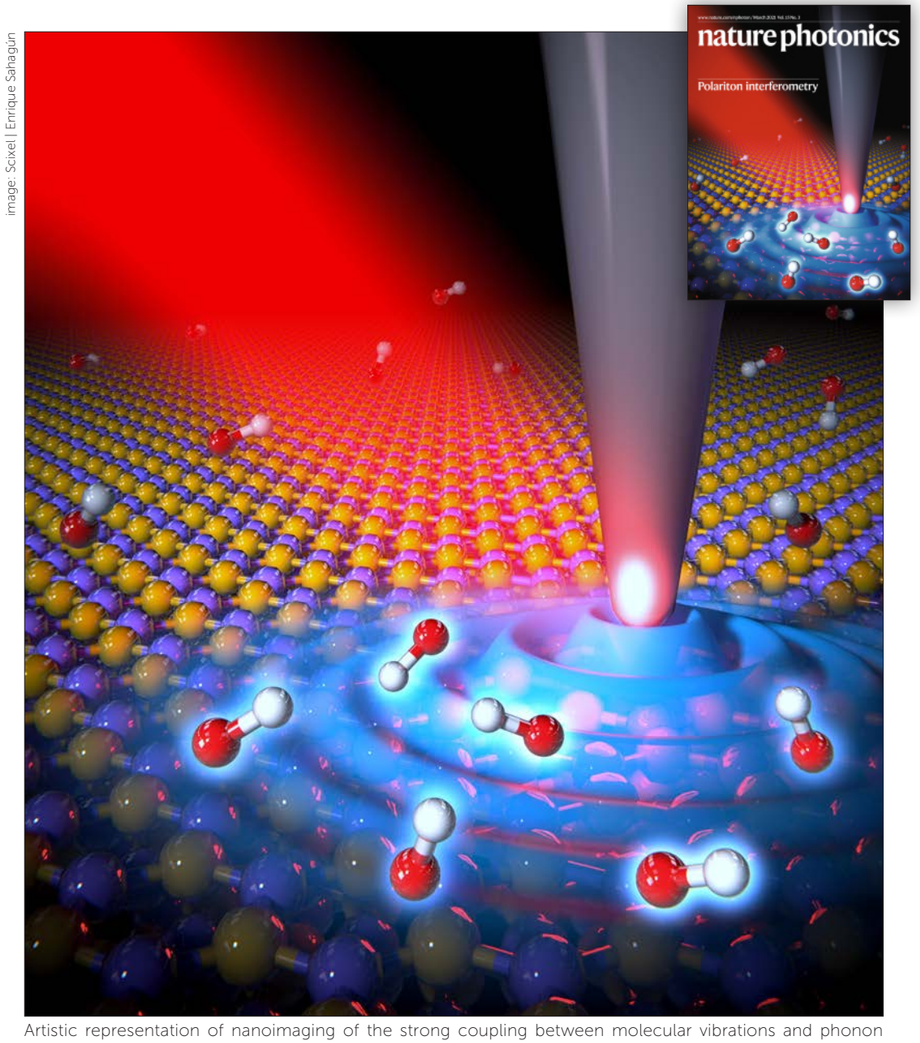
A team of researchers has just demonstrated by nanoimaging that vibrational strong coupling can be achieved between propagating phonon polaritons in thin van der Waals crystals (h-BN) and molecular vibrations in adjacent thin molecular organic layers.

Mid-infrared nanoimaging experiments were used to study the interaction of ultra-confined propagating phonon polaritons in van der Waals materials with molecular vibrations in sub-100 nm thick organic layers. Specifically, phonon-polariton interferometry was performed in thin, continuous hexagonal boron nitride layers interacting with 4,4′-bis(N-carbazolyl)-1,1′-biphenyl molecules. The researchers retrieved—in an excellent agreement—experimentally and theoretically the quasi-normal modes of the coupled system, revealing a strong coupling.

Interestingly, a numerical study predicts that few-layer h-BN layers may enable strong coupling to be reached even in the case of atomically thin molecular layers, thus underlining the potential of phonon polaritons to become a platform for ultrasensitive on-chip spectroscopy devices.

Researchers visualize a mixed light-matter state by near-field optical microscopy

image: Scixel | Enrique Sahagún



Artistic representation of nanoimaging of the strong coupling between molecular vibrations and phonon polaritons (circular waves) in a thin slab of h-BN. Nanoimaging is performed by a near-field microscope that scans a sharp tip across the sample surface. Nature Photonics cover (Nature.com/nphoton/volumes/15/issues/3)

DIPC HIGHLIGHT 2021

Probing quantum speed limits with ultracold gases

del Campo A
Physical Review Letters 126, 180603 (2021)

In recent years, the understanding of time-energy uncertainty relations as quantum speed limits has provided deep insights in nonequilibrium processes and quantum technologies. Quantum speed limits (QSLs) rule the pace at which quantum systems can change and thus have applications ranging from quantum metrology to quantum control, orthogonality catastrophe, and the limits of computation, among other relevant examples.

Quantum physics dictates the existence of Quantum Speed Limits (QSL), that impose a minimum time for a physical process to unfold. Not surprisingly, QSL have broad applications in quantum computing, quantum metrology, and other quantum technologies. And yet, their experimental study has remained elusive for decades. The work by Prof. del Campo shows how recent advances in experimental ultracold atom physics can be harnessed to probe QSL in the laboratory, further unveiling their implication in optimal control theory.

The common understanding of the uncertainty relation says that it is impossible to measure both the position and the momentum of a subatomic particle, in the same instant to unlimited accuracy. The more accurate is the measurement of the momentum, the less accurate is the measurement of the position in that instant, and vice versa.

Momentum is certainly related to time through velocity, but introducing time in the quantum realm turns everything a little bit blurry. The time-energy uncertainty relation is a fundamental result in quantum physics relating characteristic times to the inverse of energy fluctuations, Still, as Busch puts it, different types of time energy uncertainty relation can indeed be deduced in specific contexts, but that there is no unique universal relation that could stand on equal footing with the position-momentum uncertainty relation.

The modern formulation of the time-energy uncertainty relation relies on quantum speed limits that bound the minimum time for a physical process to unfold in terms of energy fluctuations. As the state of a system in quantum mechanics is represented by a vector in a linear vector space that can have an infinite number of dimensions, called a Hilbert space, quantum speed limits represent quantum dynamics geometrically, where the quantum state of a system evolves in time by sweeping a distance in Hilbert space. Therefore, quantum speed limits involve the notions of speed and distance in Hilbert space.

Quantifying the distance between the initial and time-evolving quantum states requires estimating state overlaps, which is challenging, if not unfeasible, for many-particle systems with continuous variables.

The flow of time is marked by the happening of events allowed by quantum speed limits

Image courtesy of Guy Chenu

Artistic representation of the minimum time required for a quantum state to evolve into a distinguishable state, which is encoded in the quantum speed limit (QSL). The existence of a QSL is a fundamental principle in physics and information theory. It sets the ultimate bound on the computational power of physical devices and the complexity of the universe. Thanks to advances in quantum control of ultracold quantum matter, the study of QSL is now at reach in complex many-body systems.

In spite of the fundamental nature of quantum speed limits, there is currently a lack of experimental studies probing them. Now, Adolfo del Campo theoretically proposes the experimental study of quantum speed limits with many-body systems of trapped ultracold atoms by measuring the mean atomic cloud size as a function of the evolution time.

The proposal relies on measuring the size of the atomic cloud in a given process, such an expansion or compression driven by a modulation of the trap frequency. The scaling factor can be determined by imaging the cloud size via different methods. From it, the distance traveled by the quantum state of the system in Hilbert space (Bures angle) during the evolution can be determined.

This approach circumvents the need for reconstructing a quantum state using measurements of the many-body quantum states of a continuous variable system. These results pave the way to the experimental study of the time-energy uncertainty relation and quantum speed limits in many-body quantum systems and their relation to the orthogonality catastrophe.

DIPC HIGHLIGHT 2021

Reaching the ideal glass in polymer spheres:thermodynamics and vibrational density of states

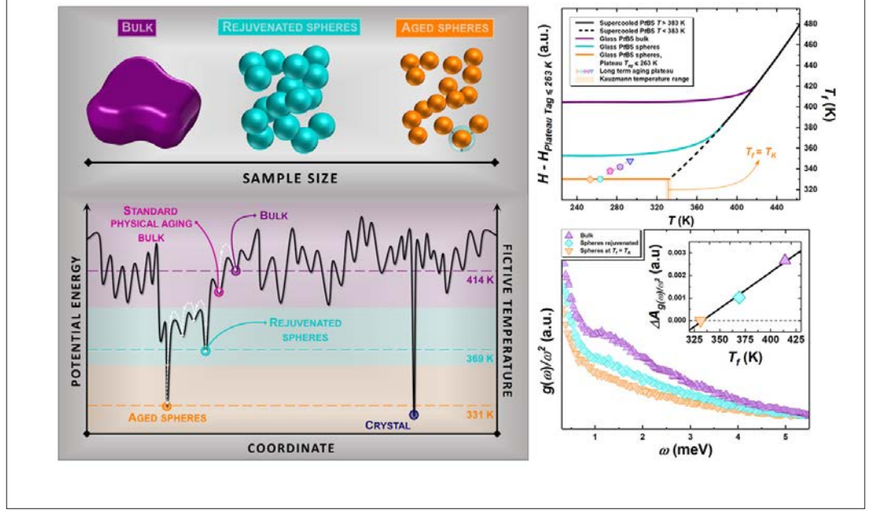
Monnier X, Colmenero J, Wolf M and Cangialosi D
Physical Review Letters 126, 118004 (2021)

Glasses, though in the solid state, differ from crystals as they exhibit no long-range order in the atomic distribution. In general, a liquid of any kind can be cooled down below its melting temperature, provided that large cooling rates are used to avoid crystallization. Further cooling leads to the formation of a glass – at a temperature addressed as glass transition temperature, T_g – whose thermodynamic state profoundly depends on its thermal history. Once in the glassy state, spontaneous evolution towards low energy states, known as physical aging, takes place.

A deep unresolved question in glass science regards the equality of the glass entropy with that of the crystal at a finite temperature, addressed as the Kauzmann temperature, T_K, implying an entropy catastrophe with the paradoxical scenario of a liquid having smaller entropy than that of the crystal at $T < T_K$. To avoid this unpalatable scenario, it has been largely debated whether a true second order thermodynamic transition, the "ideal" glass transition, at T_K takes place. An important aspect related is that, apart from the thermodynamic view, the achievement of low energy glasses may deeply affect the glass vibrational density of state (VDOS). An excess in the VDOS, addressed as the boson peak, is observed in glasses whose magnitude decreases with the energy.

Accessing low energies in bulk glasses is unfeasible due to the astronomical time scales required. Indeed the transformation of the supercooled liquid into a glass takes place at large energies and subsequent glass equilibration below T_g is extremely slow. Hence, we exploited the ability of glasses with large free interface to access low energy states. Specifically, aggregates of spheres of a polymeric glass former were aged well below their T_g and characterized by calorimetry and inelastic neutron scattering to monitor the thermodynamic state and the VDOS, respectively.

The results show that, when aged at appropriate temperatures, glassy spheres attain a thermodynamic state corresponding to an ideal glass in about one day; indicating that increasing glasses' free interface induces a tremendous reduction of the timescale to recover equilibrium. Via a relaxation process with finite timescale deep in the glassy state, this acceleration allows attaining glass energies relevant to detect a kink in the enthalpy, identified with the transformation from the standard into the ideal glass (see Figure upper right panel). In the ideal glassy state, the boson peak disappears (see Figure lower right panel), thus rendering the VDOS alike that of crystals.



(Left panel) Schematic representation of the potential energy landscape for bulk and spheres glasses, showing how deep in the in the landscape the latter system can fall. (Right upper panel) Thermodynamic plot showing the glass enthalpy of bulk and polymer spheres, the equilibrium (supercooled) line and the kink in the enthalpy at the ideal glass transformation. (Right lower panel) Reduced VDOS for bulk and polymer spheres before aging (rejuvenated) and in the ideal glass state. The inset shows the relation between the glass thermodynamic state and the VDOS.

The existence of the ideal glass is proved by aging glasses with large amount of free interface. The boson peak in the ideal glass is suppressed

DIPC HIGHLIGHT 2021

Enhancement of spin-charge conversion in dilute magnetic alloys by kondo screening

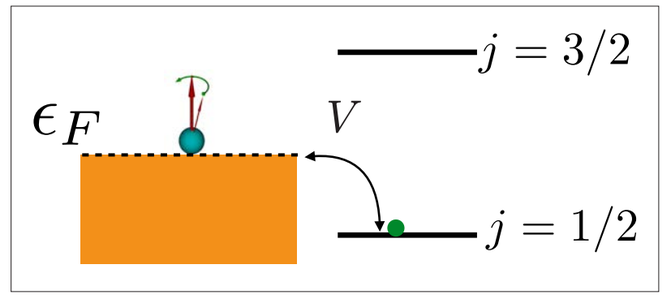
Huang C, Tokatly Ilya V. and Cazalilla MA
Physical Review Letters 127, 176801 (2021)

The importance of impurities in determining the properties of materials cannot be sufficiently understated. After all, our current information technologies are based on devices made from doped semiconductors. Indeed, semiconductors like Silicon would be boring insulators was it not because by randomly introducing impurities they can be turned into metals. Thus, exquisite control of the electric conductivity is possible in devices with metallic gates imprinted on the surface.

However, besides the electrical charge which behaves classically (except for being quantized), electrons also possess an intrinsically quantum mechanical degree of freedom, namely the spin. The field of spintronics was born out of an attempt to control the electron spin and use it for the storage and transport of (quantum) information. In recent years, the generation of spin polarized currents without relying on magnetic materials has become a major research topic. One approach relies on materials whose band structure exhibits a large spin-orbit splitting. Thus, in response to external electric fields, large spin currents can be generated (the so-called intrinsic spin Hall effect, ISHE).

However, synthesizing such materials often requires heavy elements that are scarce or hard to mine from the Earth crust. In addition, it is interesting to use heavy elements in small amounts as contaminants in order to synthesize alloys with interesting spintronic properties. For spin current generation, this relies on the extrinsic spin Hall effect (ESHE). There are two contributions to the ESHE: skew scattering and side jump. The former can be readily incorporated in a kinetic theory describing the transport of electrons in metals. The latter has been extensively discussed by many authors but, unlike skew scattering it has not been possible to account for it within a rigorous kinetic theory until the publication of our work). Instead, various heuristic approaches involving the introduction of an anomalous velocity due to the scattering of electron wave packets with heavy atom impurities have been used so far.

Along with large spin-orbit splittings, electrons in the orbitals of heavy atom impurities also experience strong correlation effects. This has been known to lead to phenomena like the Kondo effect in magnetic alloys. The latter often manifests itself as a minimum in the electrical resistivity of metals contaminated with transition metal impurities like Fe, Co, Mn, or rare earth impurities like Ce, Yb, etc. At low temperatures, this effect eventually results in the disappearance of the impurity's magnetic moment after being screened by the conduction electrons of the metal. What is left behind is often an impurity that resonantly scatters electrons at the Fermi energy.



Simplified model of a Cerium impurity in a rare earth $Ce_xLa_{1-x}Cu_6$ to which we applied our kinetic theory. The impurity is made rotationally invariant but captures the low-lying multiplet structure of Cerium impurities in the alloy. Two mutiplets with (effective) j = 3/2 and j =1/2 for the f-electron, with the j =1/2 giving rise to the Kondo effect. An addition scattering channel with j = ½ resulting from other orbitals is also included. The j =1/2 double is Kondo screened at low temperatures.

Our theory uses the density impurities as a small parameter but accounts for arbitrarily strong impurity scattering

The equations obtained in our work provide the first rigorous derivation of side jump contribution within kinetic theory. When deriving the Boltzmann equation and properly accounting for the gradient corrections, we found that gradient corrections to the collision integral readily account for the side jump mechanism. Our theory uses the density impurities as a small parameter but accounts for arbitrarily strong impurity scattering. We solved our kinetic equations and made concrete predictions for the spin Hall conductivity of rare earth alloys like $Ce_xLa_{1-x}Cu_6$, which exhibits the Kondo effect phenomenology for small x. Thus we found 1) a sizeable contribution to the ESHE entirely due to the side jump which does not depend on the interference with other scattering channels 2) A difference in the diffusion coefficients for the longitudinal and transverse components of the spin density.

DIPC HIGHLIGHT 2021

Global natural orbital functional: towards the complete description of the electron correlation

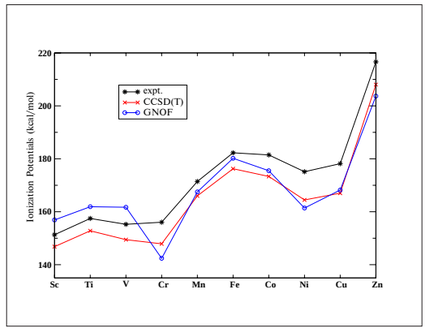
Piris M
Physical Review Letters 127, 233001 (2021)

Our current understanding of how electrons are found in atoms and molecules is based on clouds of probability. According to quantum mechanics, the probabilities of finding an electron in different regions of space can be obtained by solving the Schrödinger equation. Its solution is called the wavefunction, ψ, and the square of the absolute value of the wavefunction, $|\psi|^2$, defines the probability density function.

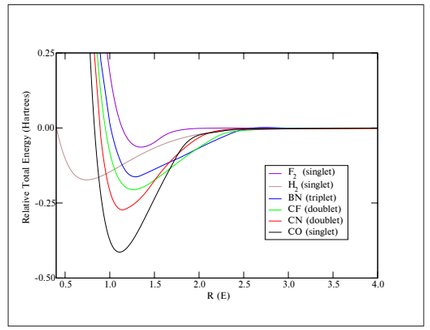
The solution of the Schrödinger equation for multielectron systems is one of the central problems in physics and is far from trivial. For the most interesting quantum mechanical systems, we don't know how to solve the Schrödinger equation. There are exceptional systems of "exact resolution" such as the free particle, the square well or the harmonic oscillator; however, for other systems, such as a many-electron atom or a molecule, we rely on various approximation methods.

Probably the most popular approaches are based on density functional theory (DFT). In DFT, the electron density completely determines a many-electron system and, in particular, the total energy turns out to be a density functional. This represents a great advantage since it avoids having to know the wave function ψ that contains much more information, significantly lowering the computational costs to solve the many-body problem. Unfortunately, attempts to construct such a functional for the total energy have not been very successful due to its strong non-locality.

Appropriate representations of the electronic structure of atoms, molecules and solids without explicit recourse to the wavefunction can alternatively be obtained by the one-particle reduced density matrix (1RDM) functional theory. The functionals currently in use are constructed in the basis where the 1RDM is diagonal which is the definition of a natural orbital functional (NOF). In NOFT, the electronic structure is described in terms of the natural orbitals and their occupation numbers. The approximate NOFs have proven to be more accurate than those of the density for systems with a significant multiconfigurational character, on one side, and scale better with the number of basis functions than correlated wavefunction methods, on the other side. Several approximate NOFs have been proposed, but they suffer from an important lack of dynamic correlation.



Ionization potentials of transition-metal atoms.



Potential Energy Curves.

An even more elegant approach for the description of electronic correlation based only on the one-particle reduced density matrix

In 2017, Mario Piris, an Ikerbasque research professor working at DIPC and UPV/EHU, proposed a new method to calculate electron correlations based on the NOF theory. To recover the dynamic correlation, second-order perturbative corrections were considered with significant results. The implementation of the method in an open-source code called DoNOF (Donostia Natural Orbital Functional) was presented three years later. Now, Piris provides the next step towards the complete description of the electron correlation. He has designed an accurate NOF for electronic systems with any spin value independent of the external potential being considered, that is, a global NOF (GNOF).

Piris limits himself to a new two-index reconstruction of the two-particle reduced density matrix for spin multiplets, and introduces the concept of the dynamic part of the occupation numbers. The emergent functional describes the complete intrapair electron correlation, and the correlation between orbitals that make up both the pairs and the individual electrons.

The results for different properties calculated this way agree extremely well with experimental data. Piris now recovers the missing dynamic correlation within the NOF theory framework only.

DIPC HIGHLIGHT 2021

Coulomb interaction, phonons, and superconductivity in twisted bilayer graphene

Cea T and Guinea F
PNAS 118, e2107874118 (2021)

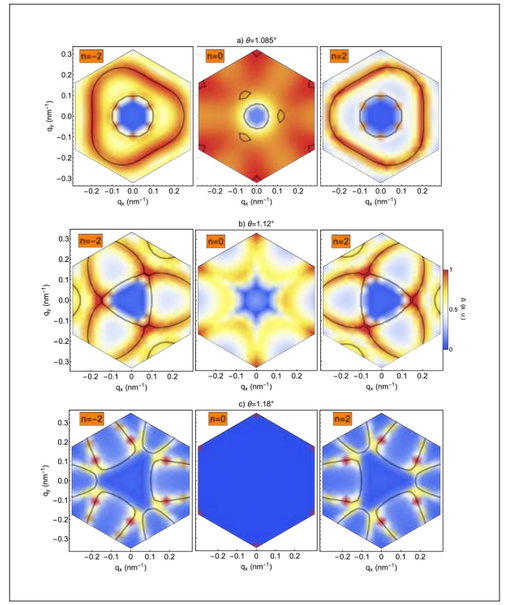
Twistology could be the study of unexpected changes or developments in stories or situations, from coups d'état to the fatherhood of Darth Vader. In condensed matter physics there is something similar, although the preferred name is twistronics (from twist and electronics). It is understood as the study of how the angle (the twist) between layers of two-dimensional materials can change their electrical properties. Materials such as twisted bilayer graphene (TBG) have been shown to have vastly different electronic behaviour, ranging from non-conductive to superconductive, that depends sensitively on the angle between the layers.

The development of superconducting devices was greatly stimulated after the acceptance of the basic theory of superconductivity proposed in 1957 by John Bardeen, Leon Cooper, and Robert Schrieffer. The authors of the BCS theory, as it is known, received the Nobel Prize for their work in 1972. The basic idea is that the electron waves in the superconducting state no longer act independently, as in Bloch's model. Instead, they are paired together at the so-called critical temperature so that their wave functions act as one unit as they interact with the crystal lattice. Moreover, all of the electron pairs move together in one collective motion, so that if any single electron is scattered by the lattice it is pulled back into the flow by its partner, and if any pair of electrons is somehow scattered off track, it is pulled back into the collective flow by all the other pairs. Since there is no scattering or inelastic collisions, there is no resistance, and the material becomes a superconductor.

The pairing interaction responsible for superconductivity in TBG has been intensively studied. Among other possible pairing mechanisms, the effect of phonons, the proximity of the chemical potential to a van Hove singularity in the density of states and excitations of insulating phases, and the role of electronic screening have been considered.

Now, Tommaso Cea and Francisco Guinea study 1 how the screened Coulomb interaction induces pairing in TBG. The researchers obtain critical temperatures of magnitude 1 to 10 K and provide estimates and trends in agreement with the experimental measurements.

The long-range Coulomb interaction, projected onto the central bands of TBG, is described by an energy scale in the range of 20 to 100 meV. As a result, this interaction modifies significantly the shape and width of the bands of TBG near the so-called first magic angle. The authors focus on low-energy excitations in TBG, including particle–hole excitations, plasmons, and acoustic phonons, analysing the way in which these excitations lead to superconductivity, by means of well-tested diagrammatic techniques.



Electronic structure and superconductivity in twisted bilayer graphene. The plots show the Fermi surfaces and peaks in the superconducting order parameter for different numbers of electrons.

The strongest interaction between electrons in twisted bilayer graphene is the long range Coulomb repulsion

The article shows that, nevertheless, this interaction induces superconductivity, due to the complex structure of the electronic bands

The scientists find that the screened Coulomb interaction allows for the formation of Cooper pairs and superconductivity in a significant range of twist angles and fillings. The tendency toward superconductivity is enhanced by the coupling between longitudinal phonons and electron–hole pairs. Importantly, scattering processes involving large momentum transfers play a crucial role in the formation of Cooper pairs.

This is another important theoretical contribution to understand superconductivity in general, and particularly in TBG.

DIPC HIGHLIGHT 2021

Simulation methods for open quantum many-body systems

Weimer H, Kshetrimayum A and Orús R
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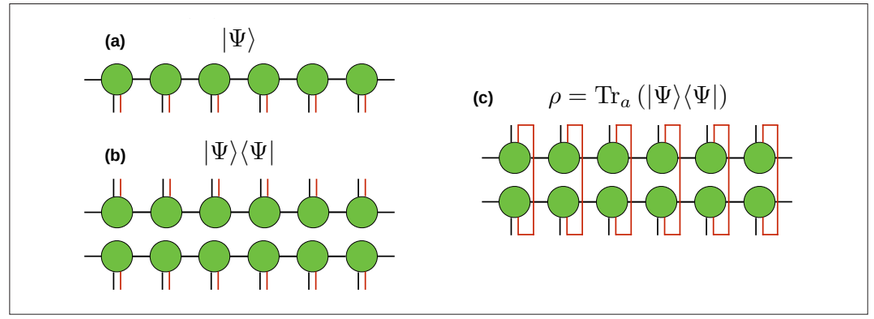
It is very difficult to obtain exact solutions to systems involving interactions between more than two bodies, using either classical mechanics or quantum mechanics. To understand the physics of many-body systems, it is necessary to make use of approximation techniques or model systems that capture the essential physics of the problem. The complexity of the problem scales exponentially with the size of the system, requiring the use of sophisticated simulation methods to obtain useful results This is compounded by the fact that no system in nature is perfectly isolated. They are constantly interacting with their environment in the form of heat transfer, decoherence, etc. Actually, all real systems are open systems.

Open quantum many-body systems have witnessed a surge of interest in recent years, chiefly for two reasons. On the one hand, these systems offer the possibility of using controlled dissipation channels to engineer interesting quantum many-body states as the stationary state of their dynamics. On the other hand, open quantum many-body systems are attractive from a fundamental perspective, as their dynamics exhibits a wide range of features not found in equilibrium systems.

Open quantum many-body systems are even harder to simulate on classical computers than closed systems, while at the same time the stationary state of an open quantum system is much easier to experimentally prepare than the ground state of a closed system. These properties make open quantum systems one of the prime candidates to show a quantum advantage of quantum simulators over classical methods within noisy intermediate-scale quantum devices. However, this requires a thorough assessment of the capabilities of classical simulation methods, which a team of researchers now provide in a new review.

The substantial effort to develop novel simulation methods to investigate open quantum many-body systems has produced a variety of numerical methods. Specifically, in this review methods for the Markovian quantum master equation (assuming a weak-coupling limit), including mean-field stochastic methods, tensor networks, variational methods, quantum Monte Carlo methods, a truncated Wigner approximation, BBGKY hierarchy equations, and linked-cluster expansions are considered.



(a) A quantum state described by a Tensor Network includes degrees of freedom for the system (black lines) and the environment (red lines). The projector (b) describes the complete system, and the trace over the environment in (c) produces a quantum state in the form of a Tensor Network capable of describing the physical system directly, by means of a reduced density matrix that can be manipulated computationally for very large systems.

Simulaiting open and noisy systems is now possible by using a variety of computational techniques, allowing for the discovery of new phases of dissipative quantum matter

While no method has yet emerged that is universally optimal for all cases, there have been several promising developments with different methods for different regimes. Even with the major technical advances recently achieved, there are still many open problems that are inaccessible with these state-of-the-art numerical techniques.

The authors come to very interesting conclusions. The first is that mean-field methods are considerably less reliable for open systems than their counterparts for closed systems, although the reason for this discrepancy is still an open question. Secondly, tensor network methods have demonstrated their ability to successfully tackle many hard problems surrounding open many-body systems and resolve long-standing open questions. A particularly interesting and promising case is that of open 2D systems, which are unexplored territory to a large extent. Finally, for the variational methods discussed in this review, there appears to be a trade-off between the formal suitability of the norm and its efficient computability.

Progress in recent years in simulating open quantum systems has brought the field to a level where one has a wide range of tools at hand to systematically make a comparison to experimental results, particularly in the context of quantum simulations. Combined with the experimental ease of preparing the steady state of an open quantum system, these are good reasons to believe that the study of strongly correlated open quantum many-body systems will become a research topic with an impact on other areas of science, such as material design and quantum computation.

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Electronic structure of molecular excited states and photophysical process: theory and applications.

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Field of molecular indicators for single atom detection in dry media, with major applications to neutrino physics and a clear potential for biomedical.

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Prediction of new topological phases and materials.

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01/07/2019–23/01/2021
Deep eutectic solvents for biomass extraction.

Dr. Fernando Javier Gomez Ruiz
01/07/2019–Present
Tailoring quantum matter far away from equilibrium.

Dr. Jens Stucker
01/09/2019–Present
Cosmology.

Dr. Tao Wang
07/10/2019–Present
On-surface synthesis of functional molecular materials.

Dr. Fernando Aguilar-Galindo Rodriguez
15/01/2020–Present
Quantum chemistry calculations of molecules adsorbed on surfaces for applications in nanophotonics including ultra-fast spectroscopy and surface-enhanced spectroscopy.

Dr. Félix Mouhat
20/01/2020–19/01/2021
Numerical calculations of tunneling conductance in the presents of the Kondo effect.

Dr. Nuno De Sousa Teixeira
03/02/2020–Present
Light scattering in disordered and nonreciprocal media.

Dr. José Ángel Martínez González
01/04/2020–31/08/2021
Investigation of the collective dynamics at intermediate length scales in liquids and glass-forming systems by molecular dynamics simulations.

Dr. Khadiza Ali
15/04/2020–04/04/2021
Condensed Matter Physics.

Dr. Rubén Rodríguez Ferradas
01/05/2020–Present
Development of new density functional approximations.

Dr. Rishav Harsh
01/06/2020–Present
Solid-state doping of two-dimensional transition metal dichalcogenides.

Dr. Mario Fernandez Pendás
01/07/2020–31/10/2021
Molecular simulations of intrinsically disordered proteins.

Dr. Helena Almazan Molina
01/08/2020–31/07/2021
Detector design and analysis for neutrino physics in the "European Spallation Source".

Dr. Mikel Odriozola Gimeno
01/08/2020–Present
Detection of SARS-CoV-2 by specific and ultra-sensitive physico-chemical techniques.

Dr. Jonás Chaves-Montero
01/10/2020–Present
Astrophysics and Cosmology.

Dr. Carlos García Fernández
01/10/2020–30/09/2021
Electronic structure, magnetism, and quantum transport in graphene nanostructures.

Dr. Jon D'Emidio
05/10/2020–Present
Quantum Monte Carlo calculations and networks of tensors.

Dr. Luis Antonio Soriano Agueda
01/11/2020–31/01/2021
Design and implementation of exchange andcorrelation functionals for the correct description of dynamic and non-dynamic correlation.

Dr. Claire Tonnelé
01/11/2020–Present
Electronic structure in molecular photophysics and optoelectronics.

Dr. Sanghita Sengupta
17/12/2020–Present
Spin physics in graphene-based nanostructures.

Dr. José María Benlloch Rodríguez
22/01/2021–Present
Development of an image reconstruction software for a full-body PET based on liquid xenon.

Dr. Uxua Huizi Rayo
25/01/2021–Present
Design, synthesis and chemical characterization of lanthanide based chiral and enantiopure metal organic frameworks for chiral Induced spin selectivity effect studies with applications to spin-polarized electron transport and enantio-selective nuclear mag.

Dr. Oihana Galparsoro Larraza
01/02–30/04/2021
Non adiabatic effects in theoretical gas-surface kinetics.

Dr. Rafael Ramis Cortés
08/02/2021–Present
Molecular dynamics of potassium channels.

Dr. John Fredy Vélez Santa
22/02/2021–21/02/2022
Experimental surface electrochemisty studies.

Dr. Rodrigo Humberto Aguilera del Toro
17/05/2021–Present
On the quest of new magnetic 2D materials.

Dr. Francisco Javier Alfaro Mozaz
17/05/2021–Present
Optically manipulating neuronal activity with nanoparticles.

Dr. Verónica Postils Ribó
01/06/2021–31/12/2021
Development and application of NLO responses in terms of diabatic states.

Dr. María Jesús Morán Plata
20/09/2021–Present
Catalysis toward platinum substrates for drug delivery.

Dr. Mihovil Bosnar
01/10/2021–Present
Postdoctoral researcher in condensed matter physics.

Dr. Pablo Fernández Menéndez
01/10/2021–Present
Development of water Cherenkov test beam experiment.

Dr. Ana Cristina Carrasco Gento
12/10/2021–Present
Bioorthogonal photocatalysis towards metal substrates.

Dr. Ricardo Ortiz Cano
16/10/2021–Present
Quantum correlations in graphene-based nanostructures.

Dr. Valerio Di Lisio
15/11/2021–Present
Non-equilibrium dynamics of amorphous polymers and other materials.

Dr. Rodrigo Voivodic
06/12/2021–Present
Cosmology — Large Scale Structure.

Dr. Nahual Carlos Sobrino Coll
16/12/2021–Present
Electronic and thermal transport through strongly correlated systems as described by density functional theory.

Research Collaborators

Dr. Mohammad Ali Aboudzadeh Barihi
01/03/2020–28/02/2021
Metal/cyclic hybrid materials for biomedical applications.

Dr. Ilya Nechaev
01/11/2020–Present
Linear response, low-energy electron scattering, and photoemission within the relativistic k.p methodology.

Dr. Yetli Rosas Guevara
01/12/2020–Present
Theory and observation of galaxy formation.

Dr. Mireia Vía Nadal
07/12/2020–30/06/2021
Research in Benchmarking of reduced density matrix functional approximations in molecules.

Dr. Luis Antonio Soriano Agueda
01/02/2021–Present
Design of interchange and correlation functionalities for the correct description of dynamic and non-dynamic correlation.

Dr. Jorge Pelegrín Mosquera
08/09/2021–Present
Development of gas handling system for NEXT experiment.

Dr. Sergio Contreras Hantke
01/12/2021–Present
Modelling of galaxy formation physics and its impact on clustering and cosmological parameters.

PhD Students

Jorge Olmos Trigo
01/10/2016–28/02/2021
Theory and modelling of topological photonic materials.

Donaldi Mancelli
03/02/2017–Present
Experimental and theoretical analysis of simple compounds under shock-wave compression.

María Blanco De Paz
27/03/2017–26/03/2021
Spin orbit interactions in photonic systems.

Juan Gurruchaga Pereda
03/04/2017–02/04/2021
Photocatalytic upconverting nanomaterials for metal based photochemotherapy.

Mikel Olano Aramburu
01/09/2017–31/08/2021
Quantum information processing with electrons and phonons in semiconductors.

Sofia Sanz Wuhl
07/09/2017–Present
Theory of quantum transport in graphene based nanostructure networks.

Raúl Guerrero Avilés
27/10/2017–26/10/2021
Adsorbing atoms and molecules on van der Waals heterostructures.

Mohammed Sabri Gamal Mohammed
01/11/2017–28/02/2021
Functional materials synthesized by surface-supported chemistry under vacuum.

Iñigo Robredo Magro
16/11/2017–15/11/2021
Looking for new fermions in conventional crystals.

Paul Dreher
08/01/2018–Present
Manipulation of collective ground states in highly correlated transition meal dichalcogenides.

Xiang Xu
21/02/2018–Present
Study of intracular functions.

José Lanuza Delgado
01/03/2018–Present
QM and QM/MM simulations of phosphate dydrolysis reactions catalized in various environments.

Joscha Kruse
01/04/2018–Present
Dynamic self-assembly of plasmonic nanoparticles in flow.

Nahual Carlos Sobrino Coll
04/04/2018–15/12/2021
Electronic and thermal transport through strongly correlated systems
as described by density functional theory.

Masoud Mansouri
20/05/2018–Present
Electronic excitations in organo metallic compounds.

Giovanni Aricò
01/07/2018–31/08/2021
Cosmological implications of dark energy.

Irene Ruiz Ortiz
01/09/2018–Present
Intrinsically disordered drug discovery.

Unai Muniain Caballero
01/10/2018–Present
Classical and ab-initio study of optical surface excitations for nanophotonics.

Auguste Tetenoire
01/10/2018–Present
Molecular dynamics simulations of femtosecond laser induced desorption
of adsorbates from metal surfaces.

Alejandro Berdonces Layunta
22/10/2018–Present
Functional materials synthesized by surface-supported chemistry under vacuum.

Sophie Espert
01/11/2018–Present
Protonic conductivity mechanism in new electrolytes based on strong acid clathrate hydrates.

María Zubiria Ulacia
01/11/2018–Present
Triplet states in PDI and related organic molecules.

Alvaro Pozo Larrocha
08/11/2018–Present
Axionic wave dark matter project.

Pablo Herrero Gómez
01/01/2019–Present
Support for NEXT project.

Xabier Telleria Allica
08/01/2019–Present
Statically screened potentials, Hookean systems and quantum dots.

Ricardo Rama Eiroa
03/12/2019–Present
Spin dynamics in patterned antiferromagnetic nanostructures.

José Aarón Rodríguez Jiménez
10/12/2019–Present
Computational chemistry in excited states. Development of density functionalities
within the framework of the theory of time-dependent density functional.

Sara Lois Cerdeira
07/01/2020–Present
Tuning the chemical properties of graphene nanostructures.

Chiara Devescovi Massussi
01/09/2020–Present
Topological phases at the frontier of electronic, optical and acoustic materials.

Daniel López Cano
01/09/2020–Present
Computational cosmology.

Miryam Martínez Vara
01/09/2020–Present
Search for double beta decay without neutrinos with the NEXT-100 detector.

Paula Andrade Sampedro
01/09/2020–Present
Computational and experimental studies on the modification of aminoacids and peptides.

Nischal Acharya
28/09/2020–Present
The environment of quasars & evolution of galaxies.

Nathaniel Andrés Capote Robayna
01/10/2020–Present
Polaritons in anisotropic van der Waals crystals.

Daniel Muñoz Segovia
01/11/2020–Present
Charge density wave in transition metal dichalcogenides.

Antonio David Subires Santana
01/02/2021–Present
Electronic and magnetic ordering in low dimensional systems.

Irian Sánchez Ramírez
01/07/2021–Present
Modeling of strongly correlated electronic systems.

Aitor Díaz Andrés
01/08/2021–Present
Photophysical processes in molecules, molecular aggregates and molecular solids.

Juan Sánchez-Camacho Sánchez
01/08/2021–Present
Development of new bioorthogonal photocatalytic catalysts for cancer therapy.

Antonio Cebreiro Gallardo
01/09/2021–Present
Nanoneuro: Quantum computational chemistry.

Kateryna Domina
01/09/2021–Present
Anomalous wave phenomena in 2D materials.

Francesco Gambino
01/09/2021–Present
Photocatalysis towards metal substrates and its applications.

Divya Jyoti
02/09/2021–Present
Impurities on superconductor.

Mohammed Loukili
15/09/2021–Present
Exploring organic chemistry under pressure with computations.

Francisco Germano Maion
27/09/2021–Present
Cosmological large scale structure.

Lurdes Ondaro Mallea
01/10/2021–Present
Research in computational cosmology.

Markos Polkas
15/10/2021–Present
PhD position in supermassive black holes and galaxy evolution.

Xabier Díaz de Cerio Palacio
01/11/2021–Present
Electronic properties of carbon-based nanostructures.

Adam Roselló Sánchez
01/11/2021–Present
Light-matter interactions in molecular systems on surfaces.

Carlo Andrea Pagnacco
15/11/2021–Present
Synthesis of cyclic polymers for biomedical applications.

Kirill Voronin
13/12/2021–Present
Nanophotonics with van der Waals crystals.

Julen Untzaga San Vicente
21/12/2021–Present
Study of wandering black holes.

Research Assistants

Xabier Díaz de Cerio Palacio
01/10/2019–31/10/2021

José María Benlloch Rodríguez
01/12/2019–21/01/2021

Aitor Calvo Fernández
01/10/2020–31/08/2021

Markel García Ibarluzea
01/10/2020–31/01/2021

Daniele Spinoso
05/10/2020–30/04/2021

Mikel García Díez
03/11/2020–28/01/2021

Haojie Guo
05/11/2020–01/02/2021

Adrián Juan Delgado
01/12/2020–31/07/2021

Irene Casademont Reig
23/01–22/05/2021

Mathias Augustin
27/01/2021–Present

Sara Pérez Sánchez
01/02–31/03/2021

Jorge Olmos Trigo
01/03/2021–31/12/2021

María Blanco de Paz
27/03/2021–Present

Róbert Trényi
01/04–30/09/2021

Juan Gurruchaga Pereda
03/04–02/06/2021

Andrés Felipe Bejarano Sánchez
06/05/2021–Present

Teresa Celaya Garmendia
17/05/2021–Present

Juan Sánchez-Camacho Sánchez
17/05–31/07/2021

José Reina Gálvez
01/06–31/08/2021

Kateryna Domina
28/06–31/08/2021

Giovanni Aricò
01/09–31/12/2021

Leire Larizgoitia Arcocha
01/09/2021–15/01/2022

Mikel Olano Aramburu
01/09/2021–Present

Sofia Sanz Wuhl
07/09/2021–Present

Ebtisam Tarek Mohammed Saeed
15/10/21–Present

Raúl Guerrero Avilés
27/10/2021–Present

Haritz Garai Marín
15/11/2021–Present

Iñigo Robredo Magro
16/11/2021–Present

Pablo Bermejo Navas
01/12/2021–Present

Joaquín Sureda Hernandez
13/12/2021–Present

Marta Costa Verdugo
15/12/2021–Present

Engineers

Jordi Torrent Collell
16/06/2018–Present

Dr. Eva Oblak
14/09/2020–Present

Dr. Rubén González Moreno
21/09/2020–Present

Dr. Ana Belén Núñez Chico
25/01/2021–Present

Technical Assistants

Beatríz Romeo Zaragozano
01/11/2018–Present

José Luis López Gómez
15/09/2020–Present

Edurne Sáenz Párraga
25/10/2021–Present

Internships

Nerea Izquierdo Oraa
UPV/EHU, Spain
01/10/2020–11/01/2021
Analysis and proposal for the improvement of corporate communication and event dissemination tools.

Lorea Sánchez Fernández de Larrea
UPV/EHU, Spain
01/10/2020–30/06/2021, 07/06–06/08/2021
Synchrotron radiation: x-ray radiation meets physics.

Joanes Basurto
UPV/EHU, Spain
26/10/2020–14/02/2021
Analysis and proposal for the improvement of corporate communication and event dissemination tools.

Jon Pérez Etxebarria
UPV/EHU, Spain
18/01–14/04/2021
Expansion of a relational database for DIPC publications, and automation of their analysis.

Asier Enrique Izu Berrade
UPV/EHU, Spain
24/05–23/07/2021
Excitonic dynamics in molecular materials.

Joan Cardona Olives
Universitat de Barcelona, Spain
01/06–31/07/2021
Free-radical C–H activation.

Aitor González Marfil
UPV/EHU, Spain
01/06–31/07/2021
Development of open-source computer vision tools for biomedical microscopy data.

Alaitz Lecuona Isasa
UPV/EHU, Spain
01/06–31/07/2021
A blue spark to shine on the origin of the universe.

Ainhoa Villoria Barcena
UPV/EHU, Spain
01/06–31/07/2021
A blue spark to shine on the origin of the universe.

Julen Aduriz Arrizabalaga
UPV/EHU, Spain
01/06–31/07/2021
The interaction landscape of amyloid-Zn2+ from molecular dynamics and QM simulations.

Cristina Oueghlani Rodríguez
UPV/EHU, Spain
02/06–31/08/2021
Installation and configuration of an OpenOnDemand server.

Blanca Delgado Galicia
Universidad Autónoma de Madrid, Spain
15/06–13/08/2021
Design of graphene-based materials for use in atomic-scale electronic devices.

Nerea Gurrutxaga Asiain
UPV/EHU, Spain
27/06–26/08/2021
Computational Cosmology and the large-scale structure of the Universe.

María José Fernández Lozano
Universidad de Valencia, Spain
28/06–27/08/2021
Controlling light at the nanoscale with plasmonic antennas.

Markel García Ibarluzea
UPV/EHU, Spain
01/07–31/08/2021
Molecular dynamics study of the calmodulin.

Guillem Vila Siles
Universitat de Gerona, Spain
01/07–01/09/2021
Computational calculation of nonlinear optical properties.

Eric Gómez Urreizti
UPV/EHU, Spain
01/07–31/08/2021
Polymer networks based on cyclic polymers.

Anthony Michael Soler
The University of Glasgow, UK
01/07–31/08/2021
Neutrino physics at the Hyper-Kamiokande detector.

Eva Moliner Adell
Universitat Politècnica de Cataluña, Spain
01/07–31/08/2021
Single ion detection to find the nature of the neutrino.

Mikel Elorza Romera
UPV/EHU, Spain
01/07–31/08/2021
Single ion detection to find the nature of the neutrino.

Xabier Belaunzaran Sanz
UPV/EHU, Spain
01/07–31/08/2021
Data-driven prediction of nanoparticle geometry in real-time.

Enrique Rozas García
Universidad Complutense de Madrid, Spain
01/07–31/07/2021, 01/09–30/09/2021
Electronic structure of magic-angle graphene superlattices.

Markel González de Txabarri Ylla
UPV/EHU, Spain
01/07–31/07/2021, 01/09–30/09/2021
Design and implementation of a new algorithm to calculate radial intracular function.

Rebeca Coentrao Da silva
UPV/EHU, Spain
01/07–31/08/2021, 13/09–08/10/2021
Putting the DIPC information screens into production.

Yara Díaz de Cerio Arzamendi
UPV/EHU, Spain
01/07–31/08/2021, 13/09–08/10/2021
Expansion of a relational database for DIPC papers and automation of their analysis.

Jorge Iván Cárdenas Gamboa
Universitat de Barcelona, Spain
01/07–31/08/2021
Computational design of synthetic routes to polytwistane nanothreads.

Juan Manuel Garzón Vela
Basque Culinary Center, Spain
01/07–31/08/2021
Gastronomy and culinary arts.

Joseba Solozabal Aldalur
UPV/EHU, Spain
15/07–30/09/2021
INFECTON.

Pablo Iván Albito Tapia
Universidad de Navarra, Spain
21/07–31/08/2021
Migration of DIPC web pages to virtual machines.

Julie Maudet
University of Nantes, France
01/09–29/10/2021
Cultural mediation and international communication.

Xabier Persona Peña
UPV/EHU, Spain
13/09–21/11/2021
Generation of automatic reports on BERC connections to ATLAS supercomputer.

Daniel Ruskov Vangelov
UPV/EHU, Spain
01/12/2022–Present
Generation of multimedia materials for the training of supercomputing users.

Undergraduate Students

Edurne Sáenz Párraga
Universidad de Alcalá, Spain
15/03–30/09/2021
Engineering in telecommunication system.

Idoia Ugarte Olcoz
UPV/EHU, Spain
12/09/2021–Present
Double degree of physics and electronic engeneering.

Sara Navarro Rodríguez
UPV/EHU, Spain
13/09/2021–Present
Doped graphene and its electronic properties in general.

Maddi Berasategi Elorza
Universitat Autónoma de Barcelona, Spain
29/09/2021–Present
Exact exchange functional for hydrogen atom and completely dissociated hydrogen molecule.
Derivation and computational implementation.

Master's Students

Aitor Díaz Andrés
UPV/EHU, Spain
01/02–31/07/2021
Theoretical chemistry and computational modeling.

Pablo Alonso Pérez
UPV/EHU, Spain
15/04–30/09/2021
Evaluation and development of deep neural networks for super-resolution of microscopy and astrophysics images.

Matteo Esposito
Università di Trieste, Italy
15/04–30/07/2021
Non-linear structure formation in non-flat universes.

Asier Rodríguez Escalante
UPV/EHU, Spain
26/04–23/09/2021
Quantum science and technology.

Arturo Loiselle
UPV/EHU, Spain
13/09/2021–Present
Enactive cognitive sciences.

Eric Gómez Urreizti
UPV/EHU, Spain
01/10/2021–Present
Synthesis of cyclic polymers.

Lorea Sánchez Fernández de Larrea
UPV/EHU, Spain
25/10/2021–Present
Nanoscience and nanotechnology.

Arturo González Morán
UPV/EHU, Spain
26/10–15/09/2021
2D Nanophotonics.

Special Assignments

Aran García Lekue
DIPC Calls for Young Researchers

Luca Salassa
DIPC Workshops and DIPC Schools

Geza Giedke and Thomas Frederiksen
DIPC Colloquia

Marek Grzelczak
DIPC Seminars

Deung-Jang Choi and Nicolás Lorente Palacios
DIPC Courses

Aitzol García Etxarri
DIPC Transdisciplinary Skills Courses

Fabienne Barroso Bujans
DIPC Summer Internships

Gender Equality Committee

Aitzol Garcia Etxarri

Amaia Arregi Buldain

Beatriz Suescun Rodríguez

David de Sancho Sánchez

Elisa Jimenez Izal

Giovanni Aricò

Luz Fernández Vicente

Maia García Vergniory

Olatz Leis Esnaola

Ricardo Díez Muiño

Silvia Bonoli

Visiting Researchers

Long visits

PhD Student Nicoletta Carabba
Universitá de Pisa, Italy
01/02–15/03/2021
Numerical simulation of many-body quantum spin networks.

PhD Student Francisco Germano Maion
Universidade de São Paulo, Pinheiros, Brazil
01/02–01/05/2021
Cosmological large scale structure.

Prof. Francesca Baletto
King's College London, UK
28/09/2020–30/03/2021, 01/04–30/06/2021
Thermal and optical properties of assembled metallic nanoparticles.

Prof. Armando Reyes Serrato
Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Ensenada, Mexico
01/02–28/06/2021
Search for chiral topological materials.

Dr. Rubén Miguel Ochoa de Zuazola
Hitachi Cambridge Laboratory, Cambridge, UK
01/01–31/01/2021, 01/03–31/03/2021, 01/07–10/08/2021
Spintronics.

PhD Student Yash Jitendra Lapasia
University of Sussex, Brighton, UK
15/03–15/05/2021
The connection between AGN and disk galaxies.

Dr. Germán Eduardo Pieslinger
CONICET, Buenos Aires, Argentina
03/01–30/06/2021
Photocatalytic drug activation.

PhD Student Nicolas Torasso
Universidad de Buenos Aires, Argentina
04/05–15/08/2021
Development and characterization of PVA membranes (electrospinning) for arsenic removal from contaminated water.

PhD Student Ece Gülfem Stücker
Istanbul University Institute of Graduate Studies in Sciences, Istanbul, Turkey
25/01–25/03/2021
Black hole evolution in a cosmological context.

Dr. Elton Gomes Dos Santos
The University of Edinburgh, School of Physics and Astronomy, Higgs Centre for Theoretical Physics, Edinburgh, UK
10/05–31/08/2021
Designing the next generation of hard-drives using two-dimensional materials.

Germán Cousillas Martínez
Munabe Ikastetxea School, Loiu, Spain
26/05–25/11/2021
The development of a Telegram bot with Atlas job administration purposes for researchers at DIPC.

Prof. Oleg V. Prezhdo
University of Southern California, Los Angeles, USA
01/06–31/08/2021
Excited state dynamics in nanoscale materials for solar energy harvesting.

Prof. Andrey Vasenko
HSE University, Moscow, Russia
01/06–31/08/2021
Superconductivity in topologically nontrivial materials.

PhD Student Maddi Berasategi Elorza
Universitat Autónoma de Barcelona, Spain
01/07–31/08/2021
Exchange and correlation energy functionals from entangled states.

Prof. Francisco José García Vidal
Universidad Autónoma de Madrid, Spain
01/07–31/07/2021
Quantum Nanophotonics.

Prof. Erez Gilad
The Unit of Nuclear Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel
02/07–02/08/2021
ESS neutron background calculations.

Dr. Linnea Pearl Soler
University of Glasgow, UK
03/07–03/08/2021
NEXT/Hyper-Kamiokande.

Prof. Paul Soler Jermyn
University of Glasgow, UK
03/07–03/08/2021
Hyper-Kamiokande, NEXT.

Dr. Aurelia Chenu
Université du Luxembourg, Luxembourg
05/07–13/08/2021
Control of open quantum systems.

Prof. Adolfo Del Campo Echevarria
Université du Luxembourg, Luxembourg
05/07–13/08/2021
Quantum systems and technologies.

Marc Querol Segura
Instituto de Física Corpuscular, Paterna, Spain
05/07–13/08/2021
NEXT-Bold, NEXT-100 and ESS.

PhD Student Nina Marta Szczotka
Wroclaw University of Science and Technology, Wroclaw, Poland
01/07–01/09/2021
Analysis of nonlinear optical properties of gas-phase molecules.

PhD Student Matthias Englbrecht
University of Innsbruck, Austria
18/07–19/10/2021
Photonic quantum information processing (in particular: indistinguishability of photons).

Prof. Francesca Ferlaino
University of Innsbruck and IQOQI, Innsbruck, Austria
22/07–29/08/2021
Novel quantum phases in ultracold dipolar gases.

Dr. Carlos Manuel Gámez Pérez
Cátedra Dr. Bofill de Ciencies y Humanitats, Gerona, Spain
01/09–30/11/2021
Complex networks for science and humanities.

Prof. Patricio Häberle
Universidad Técnica Federico Santa María, Valparaíso, Chile
01/09–01/11/2021
Growth and studi fo 2D magnetic layers on surfaces - coll.

Prof. Nicolas Laflorencie
Laboratoire de Physique Théorique, CNRS, Université Paul Sabatier, Toulouse, France
01/09–31/12/2021
Quantum magnetism and many-body localization.

Prof. Ceferino López Fernández
Instituto de Ciencia de Materiales de Madrid, Spain
01/09–30/09/2021
Disorder Photonics and AI.

PhD Student Stefano Scoditti
Universitá de Calabria, Cosenza, Italy
08/09/2021–08/03/2022
Design of miniSOG for enhance the photocatalytic properties of riboflavin.

PhD Student Carolina Andonie Bahamondes
Durham University, Centre for Extragalactic Astronomy, Durham, UK
14/09–21/11/2021
Properties and selection of obscured quasars.

PhD Student Brivael Laloux
National Observatory of Athens, Greece
15/09–15/12/2021
Obscuration of AGNs.

PhD Student Iván Ezequiel López
Univertità di Bologna, Italy
15/09–15/12/2021
Secondement of ITN Bid4Best network — work on "properties of AGN host galaxies".

PhD Student Luan Felipe Santos Martins
Federal University of Alagoas, Physics Institute, Maceió, Brazil
15/09/2021–15/03/2022
Tensor networks applied to the study of 2D heterometallic systems with exchange anisotropy.

Jozef Janovec
Brno University of Technology, Czech Republic
18/09–31/10/2021
A study of different electronic structure corrective methods used on Ni2MnGa alloy.

PhD Student Silvia Escayola Gordils
Institut de Química Computacional i Catàlisi, Universitat de Girona, Spain
01/10–30/11/2021
Theoretical study of chemical structure and reactivity of aromatic and antiaromatic excited molecular systems.

Dr. Luis Alejandro Miccio Stefancik
Instituto de Investigaciones en Ciencia y Tecnologia de Materiales, Universidad Nacional de Mar del Plata, Buenos Aires, Argentina
01/10–30/11/2021
Mestizajes — complex and neural networks modelling.

PhD Student Cameron James Brown
University of Sussex, Brighton, UK
02/10/2021–19/03/2022
Computational cosmology.

Prof. Andrey Kazansky
University of St Petersburg, Russia
03/10–03/12/2021
Retriving of the FEEL pulse with IR streaking.

PhD Student Michał Białończyk
Institute Of Theoretical Physics, Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, Kraków, Poland
11/10–15/11/2021
Exact Thermal Properties of Integrable Spin Chains.

Prof. Maxim Yurevich Kagan
Kapitza Institute of Physical Problems, Russian Academy of Sciences, Moscow, Russia
25/10–30/11/2021
Anomalous superconductivity and Coulomb correlations in novel superconductors.

Prof. Heriberto Fabio Busnengo
Instituto de Física Rosario, (CONICET - UNR), Rosario, Argentina
01/11–02/12/2021
Machine learning applied to gas-surface dynamics.

Prof. Cheol Hwan Park
Seoul National University, Seoul, South Korea
28/11/2021–28/02/2022
Topological, anomalous, and spin-Hall conductivities from effective field theory and first-principles calculations.

Short visits

Prof. Pavel Jelínek
Institute of Physics of the Czech Academy of Sciences, Praga, Czech Republic
28/06–16/07/2021
Electronic and magnetic structure of 1D molecular chains.

Dr. Alberto Rodriguez Fernandez
CNRS, Université de Bordeaux, France
29/06–01/07/2021
Quantum effects gas-surface dynamics.

Prof. Javier García de Abajo
Instituto de Ciencias Fotónicas, Castelldefels, Spain
01/07–17/07/2021
Plasmonics in atomically thin crystalline silver films.

Prof. Vladimiro Mújica Hernandez
Arizona State University, Tempe, USA
04/07–19/07/2021
Enantiospecif NMR response and chiral-induced spin selectivity.

Dr. Pierre Anthony Pantaleón Peralta
IMDEA Nanociencia, Madrid, Spain
04/07–11/07/2021
Correlated effects in graphene superlattices.

Marc Querol Segura
Instituto de Física Corpuscular, Paterna, Spain
14/02/–18/02/2021
NEXT experiment.

PhD student Daniele Spinoso
Centro de Física del Cosmos de Aragón, Teruel, Spain
14/06–18/06/2021
High-redshift Black-Hole formation in the semi-analytic model L-Galaxies.

Dr. Siddartharta Gurung López
Observatorio Astronómico de la Universidad de Valencia, Paterna, Spain
14/06–18/06/2021, 08/11–12/11/2021
Election of Ly-alpha emitters in J-PAS.

Prof. Jeremy Lim
Institut of Physics, University of Hong Kong, China
23/06–02/07/2021
Neutrino mass.

PhD Student Héctor Sainz Cruz
IMDEA Nanociencia, Madrid, Spain
04/07–11/07/2021
Graphene Flagship Core 3.

Prof. Pablo Artal Soriano
Universidad de Murcia, Spain
05/07–31/07/2021
Biomedical optics and photonics.

PhD Student David Figueruelo Hernán
Instituto Universitario de Física Fundamental y Matemáticas, University of Salamanca, Spain
12/07–23/07/2021
Collaboration inside J-PAS survey.

PhD Student Gonzalo Álvarez Pérez
Universidad de Oviedo, Spain
13/07–20/07/2021
Active tuning of hyperbolic phonon polaritons in van der Waals materials.

Prof. Andrés Felipe Santander Syro
Institut des Sciences Moléculaires d'Orsay, Université Paris-Saclay, Palaiseau, France
17/07–25/07/2021
Electronic structure of exotic states on the surface of correlated materials: STM-ARPES coupled studies.

PhD Student Amitayush Jha Thakur
Université Paris-Saclay, Gif-sur-Yvette, France
18/07–23/07/2021
Electronic structure of exotic states on the surface of correlated materials: STM-ARPES coupled studies.

PhD Student Alejandro Jimeno Pozo
IMDEA Nanociencia, Madrid, Spain
18/07–25/07/2021
Graphene flagship.

Prof. Luis Martín Moreno
Instituto de Nanociencia y Materiales de Aragón, Universidad de Zaragoza, Spain
18/07–25/07/2021
Theoretical nanophotonics.

Dr. Vahagn Mkhitaryan
Instituto de Ciencias Fotónicas, Castelldefels, Spain
24/07–07/08/2021
Plasmons in atomically thin silver structures.

Prof. Jacek Generowicz
CERN Switzerland, Ginebra, Switzerland
25/07–31/07/2021
NEXT / PETALO.

Prof. Adolfo González Grushin
Néel Institute, Grenoble, France
15/08–29/08/2021
Topological matter school.

Prof. Alexander Altland
Institute for Theoretical Physics, University of Cologne, Koeln, Germany
20/08–25/08/2021
Organizer Topological Matter School 2021.

PhD Student Ferran Jiménez Cuélliga
Institut de Química Teòrica, Universitat de Barcelona, Spain
06/09–19/09/2021
Implementation of continuous symmetry measures for the electron density in Cosymlib python library.

PhD Student Nils Hoyer
Max Planck Institute for Astronomy, Heidelberg, Germany
11/09–15/09/2021
Modelling the cosmological evolution of nuclear star clusters.

Prof. Diego Frustaglia
Universidad de Sevilla, Spain
12/09–18/09/2021
Spin dependent quantum transport.

PhD Student Eusebio Rodríguez Fernandez
Universidad de Sevilla, Spain
12/09–18/09/2021
Spin dependent quantum transport.

PhD Student Markos Polkas
National and Kapodistrian University of Athens and National Observatory of Athens, Greece
13/09–18/09/2021
Supermassive black holes and galaxy evolution.

PhD Student Julen Untzaga San Vicente
Institute of Space Sciences, Cerdanyola del Vallès, Spain
13/09–16/09/2021
Wandering black holes.

Dr. Martin Zeppenfeld
Max-Planck Institut for Quantum Optics, Garching, Germany
15/09–19/09/2021
Investigation of cold polar molecules.

Prof. Antonio Hernando Grande
Universidad Complutense de Madrid, IMA-UCM, Madrid, Spain
27/09–30/09/2021
Effect of magnetic fields on gating of neuron channels.

Prof. Guido Burkard
Fachbereich Physik, Universität Konstanz, Sweden
02/10–07/10/2021
Spin qubits in nanostructures.

PhD Student Amitayush Jha Thakur
ISMO - Université Paris-Saclay, Orsay, France
03/10–18/10/2021
Angle resolved photoemission in metal dibromides.

Prof. Guinievere Kauffmann
Max Planck Institute for Astrophysics, Garching, Germany
03/10–27/10/2021
Star formation as a function of the internal environment within a galaxy.

Prof. Simon White
Max Planck Institute for Astrophysics, Garching, Germany
03/10–27/10/2021
Cosmological structure formation.

Prof. Giorgio Benedek
Università di Milano-Bicocca, Milano, Italy
04/10–29/10/2021
Dynamics of low-dimensional systems.

PhD Student Helene Müller
Max Planck Institute for the Science of Light, University of Erlangen-Nürnberg, Erlangen, Germany
19/10–21/10/2021
Correlated electronic states in two dimensional quantum materials.

Prof. Paulo Jose Monteiro
University of California at Berkeley, El Cerrito, California, USA
02/11–06/11/2021
Concrete science and engineering.

Dr. Mélanie Chevance
Heidelberg University, Heidelberg, Germany
07/11–14/11/2021
The origins of stars and clusters during galaxy formation.

Prof. Diederik Kruijssen
Heidelberg University, Heidelberg, Germany
07/11–14/11/2021
The origins of stars and clusters during galaxy formation.

PhD Student Daniele Spinoso
Universidad de Zaragoza, Spain
08/11–26/11/2021
Modelling the formation and evolution of supermassive BHs in the semi-analytic model L-galaxies.

PhD Student Alberto Torralba Torregrosa
Observatorio Astronómico de la Universidad de Valencia, Paterna, Spain
08/11–12/11/2021
J-PAS.

Prof. Andrey Borissov
Institute of Molecular Sciences in Orsay, France
09/11–12/11/2021
Strong field photoemission, quantum approaches in plasmonics.

Prof. Antonio Hernando Grande
Universidad Complutense de Madrid, IMA-UCM, Madrid, Spain
09/11–16/11/2021
Effect of magnetic fields on gating of neuron channels.

PhD Student Olga Matveeva
Moscow Institute of Physics and Technology National Research University, Moscow, Russia
13/11–06/12/2021
Molybdenum oxide plasmonics.

Dr. Facundo Rodriguez
Instituto de Astronomía Teórica y Experimental, Córdoba, Argentina
13/11–20/11/2021
Large-scale structure of the universe.

Prof. Nataliya Pugach
Moscow Institute of Electronics and Mathematics, HSE University, Moscow, Russia
14/11–25/11/2021
Anomalous Josephson junctions.

Prof. Rosa López Gonzalo
Insitute of Interdisciplicary Physics and Complex Systems, Palma de Mallorca, Spain
24/11–29/11/2021
Quantum consensus dynamics by entangling Maxwell Demon.

PhD Student Gonzalo Álvarez Pérez
Universidad de Oviedo, Spain
28/11–02/12/2021
Active polariton tuning of hyperbolic phonons in van der Waals materials.

Prof. Antonio Hernando Grande
Universidad Complutense de Madrid, IMA-UCM, Madrid, Spain
29/11–04/12/2021
Effect of magnetic fields on gating of neuron channels.

Dr. Khadiza Ali
Chalmers University of Technology, Gothenborg, Göte, Sweden
02/12–17/12/2021
Investigating vanderwall Ferromagnet using MOKE and low temperature STM/STS.

Personnel

Administration

Dr. Olatz Leis Esnaola
Director of Economics & Finance and Project Management

Beatriz Suescun Rodríguez
Director of Administration, Human Resources and Legal Area

Karmela Alonso Arreche
Administrative

Marimar Álvarez San Martín
Administrative

Juan Burgos Jimenez
Maintenance Manager

Amaia Etxaburu Munduate
President's Assistant

Nerea Fariñas Conde
Administrative

Maite Gutiérrez Quesada
Project Management and Administration Technician

Francisco López Gejo
Technology Transfer Manager

Natasha Nedashkivska
Administrative

Yannick Sáenz Augusto
Administrative

María Tarazona Lorente
Administrative

Outreach

Dr. Nora González Lacunza
Outreach Manager

Dr. Amaia Arregi Buldain
Outreach Officer

Valentina Rodríguez Castro
Outreach Technician

Computing Center

Dr. Txomin Romero Asturiano
Computing Center Director

Belén Isla Rodriguez
HPC Systems Manager

Jose Caballero Tobajas
HPC Resources Technician

Luz Fernández Vicente
Operation and Help Desk Manager

Daniel Franco Barranco
HPC Resources Technician

Diego Lasa Goicuría
Computing Services Manager

Carmen Martín Pulpón
Systems, Security and Networks Manager

Seminars

1 Application of hybrid quasiparticles in the next generation of integrated opto-electronics *
29/01/2021
Ivan Pshenichnyuk
Skolkovo Institute of Science and Technology, Moscow, Russia

2 Methods and applications of quantum control *
11/02/2021
Yue Ban
UPV/EHU, Donostia/San Sebastián, Spain

3 Quantum parameter estimation — from fundamentals to applications *
12/02/2021
Manuel Gessner
Ecole Normale Superieure, Paris, France

4 ICSP webinar I: To knot and not: graph theory and chemical probing unravel SARS-CoV-2 RNA frameshifting element structures *
23/02/2021
Tamar Schlick
New York University, New York, USA

* Online attendance, ** Hybrid attendance

5 ICSP webinar II: Nanomechanics of microbial infections:
from single proteins to single cells *
23/02/2021
Raúl Pérez-Jiménez
CIC nanoGUNE, Donostia/San Sebastián, Spain

6 Synthesizing topological phases in atomic and electronic quantum matter *
25/02/2021
Tobias Grass
Instituto de Ciencias Fotónicas, Barcelona, Spain

7 From plasmon-mediated molecular spectroscopy
to molecular electro-optics and quantum technologies *
26/02/2021
Tomas Neuman
Institut de Physique et Chimie des Matériaux de Strasbourg, France

8 Born to be different: how structural changes affect catalytic activity *
26/03/2021
Francesca Baletto
King's College London, UK

9 Probing the robust signatures of fragile topology *
09/04/2021
Valerio Peri
ETH, Zurich, Switzerland

10 Exploring quantum properties in 2D organic materials *
23/04/2021
Ignacio Piquero-Zulaica
Technical University of Munich, Garching, Germany

11 Magnetism, spin dynamics and transport at the nanoscale *
22/04/2021
Manuel dos Santos Dias
Peter Grünberg Institut, Forschungszentrum Jülich, Germany

12 Explosive astronomical transients and multimessenger astronomy *
30/04/2021
Christina Thöne and Antonio de Ugarte Postigo
HETH/IAA-CSIC, Granada, Spain

13 Creative destruction lab: from quantum research to quantum startups *
06/05/2021
Sam Kearney
CDL Quantum Stream, Toronto, Canada

14 Membrane mechanics and dynamics: from vitro to vivo *
14/05/2021
Adai Colom Diego
Biofisika Institute, UPV/EHU, Bilbao, Spain

15 Optical excitations with free electrons: challenges and opportunities *
15/07/2021
Javier García de Abajo
ICFO-Institut de Ciencies Fotoniques, Barcelona, Spain

16 Neutron science and applications: from clean energy
and homeland security to neutrino physic *
16/07/2021
Erez Gilad
Ben Gurion University, Beerseba, Israel

17 QUANTUM MATERIALS AND DEVICES SEMINARS
Carbon with a twist: electrons and phonons in moiré graphene bilayers *
15/09/2021
Hector Ochoa
Columbia University, New York, USA

18 Ultracold polyatomic molecules: a quantum toolbox for fundamental investigation *
16/09/2021
Martin Zeppenfeld
Max-Planck Institut for Quantum Optics, Garching, Germany

19 QUANTUM MATERIALS AND DEVICES SEMINARS
Sublattice-pseudospin-paramagnon mediated superconductivity
in magic angle twisted bilayer graphene *
29/09/2021
Chunli Huang
University of Texas, Austin, USA

20 Quantum computing with spins in semiconductors *
04/10/2021
Guido Burkard
University of Konstanz, Germany

21 QUANTUM MATERIALS AND DEVICES SEMINARS
Quantum metric in Hermitian and pseudo-Hermitian systems *

13/10/2021

Giandomenico Palumbo

Dublin Institute for Advanced Studies, Ireland

22 From simplicity to universality and undecidability *

15/10/2021

Gemma de las Cuevas

University of Innsbruck, Austria

23 QUANTUM MATERIALS AND DEVICES SEMINARS
Landau's Fermi liquids in disguise *

27/10/2021

Michele Fabrizio

International School for Advanced Studies, Trieste, Italy

24 Multiscale X-ray tomography of construction materials **

05/11/2021

Paulo Monteiro

University of California, Berkeley, USA

25 How do stars form? from cold gas to hot bubbles **

10/11/2021

Mélanie Chevance

Heidelberg University, Germany

26 QUANTUM MATERIALS AND DEVICES SEMINARS
Superconductivity in graphene-based systems *

10/11/2021

Tero T. Heikkilä

University of Jyväskylä, Finland

27 Stellar clustering connecting the formation and evolution of galaxies
to the formation and evolution of us **

12/11/2021

Diederik Kruijssen

Heidelberg University, Germany

28 Site-specific selectivity of stepped pt surfaces
for methane dehydrogenation at low temperatures **

17/11/2021

Heriberto Fabio Busnengo

Instituto de Física Rosario, Argentina

29 QUANTUM MATERIALS AND DEVICES SEMINARS
Quantum annealing: dissipative dynamics and shortcuts to adiabaticity *

24/11/2021

Procolo Lucignano

Università di Napoli Federico II, Italy

30 Quantum consensus dynamics by entangling maxwell demon **

26/11/2021

Rosa López

Instituto de Física Interdisciplinar y Sistemas Complejos, Palma de Mallorca, Spain

31 QUANTUM MATERIALS AND DEVICES SEMINARS
Nonlinear response in strongly correlated systems *

08/12/2021

Robert Peters

Kyoto University, Japan

32 Multi-gap topology of phonons **

09/12/2021

Bartomeu Monserrat

University of Cambridge, UK

Workshops

Other Workshops

Conference on Quasielastic Neutron Scattering and Workshop on Inelastic Neutron Spectrometers (QENS/WINS 2021)

May 17- 20, 2021
Online
http://qens-wins2021.dipc.org/

Organizing Committee
Arantxa Arbe (CFM-MPC)
Juan Colmenero (CFM-MPC, DIPC)

The QENS/WINS 2021 event constitutes the 14th Edition of the QENS series and the 9th of the WINS workshops. The main purpose of the QENS series is to cover the broad spectrum of scientific activities related with the investigation of dynamical processes using quasielastic neutron scattering techniques (accessing both, frequency and time domains). QENS offers a platform for discussion and exchange of scientific ideas among the experts in this field, and a general overview to newcomers about the capabilities of QENS in exploring atomic and molecular motions and relaxation processes of novel materials and diverse systems. In particular, this edition of the conference explores and exploits the potential synergies between different methods (including experimental techniques and simulations), in order to face diverse scientific challenges emerging in different research fields. WINS – Workshop on Inelastic Neutron Spectrometers–covers innovative aspects of neutron instrument design. Progresses on new spectrometer projects are presented, following the theme: "New idea, New concept, New design, New instrumentation for New sciences".

The conference was supported by a 'moodle' where all information about the meeting was available, and forums were open where participants could pose / answer questions to the presenters and exchange ideas throughout the meeting.

From 14:00h to 16:30h Central European Summer Time, four lectures of 30 minutes each were given by experts in different fields. The central 30-minutes slot was dedicated to promote interaction among the attendants, participating in a topical discussion or live chatting with colleagues. Particularly lively were the topical discussions: the themes varied every day, covering: neutron scattering experiments after Covid, sample environment, software and data analysis, needs for future instrumentation, and education and training.

With a very high participation level in the conference, the QENS/WINS community showed to be very active and still highly motivated despite the current difficulties posed by Covid. The nationalities were broadly distributed among 21 countries, being the highest participation from German scientists (48), followed by Spain (23) France and USA (22 each). The scientific contributions demonstrated again the great capabilities of QENS in very diverse areas (like biology, soft matter, energy, magnetism, medicine, energy). Important recent advances in neutron technologies, very important for the whole community, were also presented.

Invited Speakers
Anna Stradner (Lund University, Sweden)
Jeremy C Smith (University of Tennessee/Oak Ridge National Laboratory, USA)
Francesco Piscitelli (European Spallation Source ERIC, Lund, Sweden)
Ana Raquel Benetti (University of Copenhagen, Denmark)
Bruce D Gaulin (McMaster University, Hamilton, Canada)
Anne AY Guilbert (Imperial College London, UK)
Maths Karlsson (Chalmers University of Technology, Gothenburg, Sweden)
Sanat K Kumar (Columbia University, NY, USA)
Maria Paula Marques (University of Coimbra, Portugal)
Umbertoluca Ranieri (Universitá Roma La Sapienza, Italy)
Götz Schuck (Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany)
Letizia Tavagnacco (Universitá Roma La Sapienza, Italy)
Takeshi Yamada (Neutron Science and Technology Center, Ibaraki, Japan)
Yang Zhang (University of Illinois at Urbana-Champaign, USA)
Markus Appel (Institute Laue-Langevin, Grenoble, France)
Pascale P Deen (European Spallation Source ERIC, Lund, Sweden)
Michael Monkenbusch (Forschungszentrum Jülich, Germany)
Gøran Nilsen (ISIS Neutron and Muon Facility, Rutherford Appleton Laboratory, Didcot, UK)
Félix Jiménez Villacorta (ESS-Bilbao, Spain)

Nanoneuro 2021

June 23, 2021
Online
https://ntc.columbia.edu/nanoneuro2021/

Organizing Committee
Aitzol Garcia-Etxarri (DIPC, Ikerbasque)
Rafael Yuste (Columbia University, DIPC)

On Wednesday June 23rd 2021, we held the 13th NTC symposium of the NeuroTechnology Center at Columbia University: NanoNeuro 2021. This is a multidisciplinary symposium at the crossroads of the nanoscale and neural sciences, organized by the NeuroTechnology Center at Columbia University and the Donostia International Physics Center (DIPC), supported by the Kavli Foundation.

Due to Covid-19, it was held as an online symposium.
The symposium featured talks from leaders in both nanoscience and neuroscience and covered topics ranging from novel imaging techniques to the development of nanomaterials to aid in neural growth and repair. It is our hope that this multidisciplinary meeting of the minds helped foster scientific cross pollination and expand the horizons of both disciplines and beyond.

Invited Speakers
James Delehanty (US Naval Research Laboratory, USA)
Jonathan Owen (Columbia University, USA)
Eric Hosy (Bordeaux University, France)
Chris Xu (Cornell University, USA)
Tim Harris (HHMI Janelia, USA)
Polina Anikeeva (MIT, USA)
Ander Ramos-Murguialday (University of Tübingen, Germany)
Zhenan Bao (Stanford University, USA)

The Science of the Horsemen of the Apocalypse: A Scientific Approach to the Existential Risks of Humanity

July 12-14, 2021
Online and in person
Miramar Palace, Donostia/San Sebastián
https://uik.eus/en/la-ciencia-de-los-jinetes-del-apocalipsis-una-aproximacion-cientifica-los-riesgos-existenciales-de

Organizing Committee
Juan Ignacio Pérez Iglesias (UPV/EHU)
Ricardo Díez Muiño (DIPC, CFM)

The Covid-19 pandemic has shown that there are phenomena that can put the very existence of Humanity at risk. A pandemic caused by a virus, whose effects are not even the most devastating we can imagine, has caused hundreds of millions of infections, tens of millions of sick people, and millions of deaths. But it could have been worse. What`s more, epidemiology and virology specialists have been warning of the very real possibility of even more devastating pandemics.

Pandemics are not the only threat we may have to face. There are others, of different character (extra planetary, geological, bacteriological, environmental, geopolitical and others) whose possible materialization should not be ruled out. In this Summer Course we have intended to address these threats from a scientific perspective, and we have assessed nature, the real risk, its perception by human beings and the best possible approach to these phenomena.

Invited Speakers
Briones-Llorente C (CSIC-INTA, Spain)
de Murieta-Zugadi ES (BC3, Spain)
Bustince-Sola H (UPNA, Spain)
López-Goñi I (Universidad de Navarra, Spain)
Alkorta-Calvo I (UPV/EHU, Spain)
Zamora-Bonilla J (UNED, Spain)
Mulet-Salort JM (UPV, Spain)
Cuevas-Urionabarrenechea JAM (UPV/EHU, Spain)
de la Fuente MM (Universidad de Deusto, Spain)
Martinez-Mazaga U (Euskampus Fundazioa, Spain)
Barrado-Izagirre N (UPV/EHU, Spain)

IDS Online Workshop 2021 (IDS2021)

September 6-9, 2021
Online
http://ids2021.dipc.org/

Organizing Committee
Silvina Cerveny Murcia (Centro de Física de Materiales CSIC-UPV/EHU)
Ranko Richert (Arizona State University-ASU)
Catalin Gainaru (Fakultät Physik, Technische Universität Dortmund)

The dielectric properties of materials play a fundamental role in describing physical phenomena in many branches of modern science, technology, and engineering. The International Dielectric Society regularly organize a biennial meeting at which the results in the field are discussed, with the aim of better understanding the underlying physical processes founded in diverse types of macromolecules. This year the event was online due to Covid restrictions. There were 100 participants from different countries with diverse backgrounds (from universities and research institutes to companies). All contributions were grouped into eight sessions, and each session contained invited and oral presentations related to different areas where dielectric spectroscopy has relevance.

Invited Speakers
Birte Riechers (Roskilde Universitet, Denmark)
Karolina Adrjanowicz (Institute of Physics and SMCEBI, University of Silesia, Poland)
Tina Hecksher (Roskilde University, Denmark)
Jan Swenson (Chalmers University, Sweden)
Michael Vogel (Darmstadt University, Germany)
Larisa Latypova (The Hebrew University of Jerusalem, Jerusalem, Israel)
Airat Khamzin (Kazan Federal University, Russia)
Philipp Münzner (Fakultät Physik, Technische Universität Dortmund, Germany)
Ciprian Iacob (The Pennsylvania State University, USA)
Florian Pabst (Darmstadt University, Germany)
Simone Capaccioli (University of Pisa, Italy)
Erik Thoms (Arizona State University, USA)
Daniel M. Tong (Centro de Física de Materiales, Spain)
Malgorzata Jasiurkowska-Delaporte (Institute of Nuclear Physics, Polish Academy of Sciences, Poland)
Koji Fukao (Ritsumeikan University, Tokio, Japan)
Mohamed Kolmangadi (Bundesanstalt für Materialforschung und -prüfung (BAM), Germany)

Annual DIPC-UPV/EHU Quantum Workshop 2021

October 8, 2021
UPV/EHU Leioa Campus, Bilbao
http://dipc.ehu.es/giedke/eusqutech21.html

Organizing Committee
Enrique Rico (UPV/EHU, Ikerbasque)
Geza Giedke (DIPC, Ikerbasque)
Michele Modugno (UPV/EHU, Ikerbasque)
Roman Orus (DIPC, Ikerbasque)

The aim of the workshop is to provide a forum for exchanging ideas and fomenting collaboration for and between the groups working on or in fields related to quantum science and technology. By bringing together researchers (professors, postdocs, and students) from at least 14 different groups from UPV/EHU, CFM, and DIPC and fostering animated discussions after the talks, in the breaks and in an hourlong poster session, we think that we achieved the aim. The next installment of the workshop is planned in Donostia in 2022.

Invited Speakers
Juanjo García-Ripoll (CSIC IFF, Spain)
Dario Bercioux (DIPC, Ikerbasque, Spain)
Jorge Casanova (UPV/EHU, Ikerbasque, Spain)
Deung-Jang Choi (CSIC- CFM, Ikerbasque, Spain)
Fernando de Juan (DIPC, Ikerbasque, Spain)
Ricardo Díez Muiño (DIPC, Spain)
Igor Campillo (Euskampus, Spain)
Maxim Ilyn (CFM, Spain)
Mikel Iraola (DIPC, Spain)
Jens Siewert (UPV/EHU, Ikerbasque, Spain)

DIPC — Milano Bicocca Neuroscience Workshop

October 26-27, 2021
Donostia International Physics Center, Donostia/San Sebastián

Organizer
Luca Salassa (DIPC, Ikerbasque)

The workshop brought together researchers of the University of Milano Bicocca, the Donostia International Physics Center and other research institutes located in the Basque Country to discuss common interests in the field of neuroscience and to open new opportunities for international collaboration.

Invited Speakers
Diez Muiño R (DIPC, Spain)
Arganda-Carreras I (UPV-EHU, DIPC, Ikerbasque, Spain)
De Sancho D (UPV-EHU, DIPC, Spain)
Lopez X (UPV-EHU, DIPC, Spain)
Garcia Extarri A (DIPC, Ikerbasque, Spain)
Bergara A (UPV-EHU, DIPC, Spain)
Leonardo A (UPV-EHU, DIPC, Spain)
Salassa L (UPV-EHU, DIPC, Ikerbasque, Spain)
Barroso F (DIPC, Ikerbasque, Spain)
Sanchez-Cano C (DIPC, Ikerbasque, Spain)
Yuste R (DIPC, University of Columbia, Ikerbasque, USA)
Carril M (Biofisika, Ikerbasque, Spain)
Martin A (Achucarro, Ikerbasque, Spain)
Ruiz-Cabello J (CIC biomaGUNE, Ikerbasque, Spain)
Grzelczak M (CFM, DIPC, Spain)
Prosperi D (University of Milano Bicocca, Italy)
Masserini M (University of Milano Bicocca, Italy)
Re F (University of Milano Bicocca, Italy)
Chirico G (University of Milano Bicocca, Italy)
Colombo M (University of Milano Bicocca, Italy)
Mantegazza F (University of Milano Bicocca, Italy)
Corbo C (University of Milano Bicocca, Italy)
Vescovi A (University of Milano Bicocca, Italy)
Campione M (University of Milano Bicocca, Italy)
Mantecca P (University of Milano Bicocca, Italy)
Simonutti R (University of Milano Bicocca, Italy)
Cavaletti G (University of Milano Bicocca, Italy)
Di Valentin C (University of Milano Bicocca, Italy)

QNS-DIPC Joint Workshop on Quantum Control and Quantum Technologies

November 8-9, 2021
Online

Organizing Committee
Deung-Jang Choi (MPC, DIPC, Ikerbasque)
Nicolas Lorente (CFM, DIPC)
Ricardo Díez Muiño (CFM, DIPC)
Andreas Heinrich (QNS, Korea)

In the on-going framework of the memorandum of understanding (MoU) signed between DIPC and QNS, this workshop consisted of 5 half-hour talks for DIPC and 5 for QNS, after a brief introduction by Prof. Andreas J. Heinrich (director of the Center for Quantum Nanoscience, QNS) and Dr. Ricardo Díez Muiño (director of the Donostia International Phsyics Center, DIPC). The aim of the talks was to show the status of the collaboration initiated with the signing of the MoU and to foster new possible contacts by showing recent research by QNS and DIPC groups in the different fields of quantum science. We managed to exchange our research activities and stimulated ideas to deepen and continue our strong collaborations.

Invited Speakers
Soohyon Phark (QNS, Korea)
Yujeong Bae (QNS, Korea)
Christoph Wolf (QNS, Korea)
Fabio Donati (QNS, Korea)
Luciano Colazzo (QNS, Korea)
Nicolas Lorente (CFM, DIPC, Spain)
Adolfo del Campo (DIPC, Spain)
Geza Giedke (DIPC, Ikerbasque, Spain)
David Casanova (DIPC, Ikerbasque, Spain)
Roman Orus (DIPC, Ikerbasque, Spain)

Mestizajes — IV Encuentro Internacional sobre Literatura y Ciencia

November 22-24, 2021

Donostia International Physics Center, Donostia/San Sebastián

http://dipc.ehu.es/mestizajes/

Organizing Committee

Gustavo Ariel Schwartz (CFM, DIPC)

Aitzol García-Etxarri (DIPC, Ikerbasque)

Silvina Cerveny (CFM, DIPC)

Carlos Gámez (DIPC)

The IV Meeting on Literature and Science – A transdisciplinary approach to beauty from Science, Art and Literature was an exceptional opportunity for the participants to mix with scientists, writers, artists and other people from different fields to interact, discuss and explore a broader vision of the world, science and culture. The meeting addressed, from multiple perspectives, issues that have to do with beauty, aesthetic perception and its relevance in Art, Literature and Science. The relationship between beauty and aesthetic pleasure was debated as well as the links between symmetry and beauty; the role of symmetry in theoretical physics; the evolutionary development of the aesthetic sense and its biological bases, among other topics. We also addressed questions such as: what makes a painting, a novel or a theory beautiful to us? How much objective and subjective are there in beauty? What happens in our brain when we appreciate something beautiful? Can science help us understand beauty? Are there universal principles for aesthetic appreciation? Can a mathematical proof be beautiful?

Invited Speakers

Luis Martínez Otero (Instituto de Neurociencias de Alicante, Spain)

Albert Flexas (Universitat de les Illes Balears, Spain)

Candelas Gala (Wake Forest University, Wiston – Salem, USA)

Juan Luis Suarez (Western University, London, Canada)

José Edelstein (Universidad de Santiago de Compostela, Spain)

Melissa Murray (University College, Cambridge, UK)

XIV International Ontology Congress
Natural Determinism and Free Will

September 28-October 2, 2021
Facultad de Educación, Filosofía y Antropología, Museo Chillida-Leku, Donostia/San Sebastián
October 4, 2021
CCCB, Barcelona
October 14, 2021
Funcación Paideia Galiza, A Coruña
www.ontologia.info

Organizing Committee
Víctor Gómez Pin (UAB, Coordinator)
Bárbara Jiménez Pazos (UPV-EHU, Secretary)
Gotzon Arrizabalaga Pikabea (UPV-EHU, Collaborator)
Juan Ramón Macuso (Treasurer)

As planned, the XIV International Ontology Congress was inaugurated at Chillida-Leku Museum on the 28th of October 2021 and the San Sebastián sessions were closed in the same place on October the 2nd.

We are pleased to have had all the planned participants. Some of them were online due to well-known circumstances. Specifically, among others, Gerardus 't Hooft (honorary president of this edition of the congress, Nobel Prize in Physics) and Frank Wilcek (Nobel Prize in Physics); the female philosophers Elena Partene, Silvia de Bianchi, Nathalie Gontier and Concha Roldán (unfortunately, six months prior to the beginning of this edition of the congress, two internationally-renowned female philosophers cancelled their participation due to health issues); and Simon Kochen (central personality in the reflection on the philosophical implications of contemporary physics).

On October the 4th, at the CCCB in Barcelona, an open discussion was held with David Wallace (a central personality in quantum theory known as the Multiverse).

On October 14th, a debate on artistic creation and artificial intelligence was held at the Paideia-Galiza Foundation in A Coruña, with the participation of the eminent artificial intelligence researcher Humberto Bustince and the Jakiunde researcher Javier Echeverría.

Having all these events in mind, we believe that the congress has fulfilled its main objectives. As traditionally on previous editions of the congress, in the closing session held in San Sebastián at the Chillida-Leku Museum, the topic of the upcoming 2023 XV edition of the congress was announced, coinciding with the 30th anniversary of the founding of the congress: An attempt will be made to establish the state of the art around the problem of human singularity in the light of contemporary disciplines, such as genetics, quantum measurement theory and deep learning.

Invited Speakers
Gerardus 't Hooft, Nobel Prize in Physics. Honorary President. (Utrecht University, Holland)
Simon Kochen (Princeton University, USA)
Steen Rasmussen (Center for Fundamental Living Technology / University of Southern Denmark)
Frank Wilczek, Nobel Prize in Physics (College of liberal Arts and Science. Arizona State University, USA)
Nathalie Gontier (University of Lisbon, Portugal)
Elena Partene (ENS Paris, France)
Tim Maudlin (New York University, USA)
David M. Wallace (University of Pittsburgh, USA)
Silvia de Bianchi (University of Milan, Italy)
Concha Roldán (CSIC, Spain)
Carl Hoefer (Universitat de Barcelona, Spain)
Juan Luis Arsuaga (Museo de la Evolución Humana, Burgos, Spain)
Alberto Cordero (CUNY, USA)
Javier Echeverría (JAKIUNDE, Spain)
Félix Goñi (University of the Basque Country, Spain)
Javier Tejada (Universidad de Barcelona, Spain)

Nanophotonics of 2D Materials, N2D 2021

November 8-12, 2021
Centro de Ciencias de Benasque Pedro Pascual, Benasque
http://benasque.org/2021n2d/

Organizing Committee
Alexey Nikitin (DIPC, Ikerbasque, Spain)
Tony Low (University of Minnesota, USA)
Luis Martín-Moreno (INMA, Spain)

Over the past decade, there is a growing research activity on light-matter interactions in atomically thin materials, such as graphene, topological insulators, thin polar and semiconducting layers and other van der Waals materials, including their heterostructures. Nanophotonics of 2D materials (N2D) aims at the exploration of their optical phenomena and in providing a setting where researchers from diverse fields can convene; classical and quantum optics; excitons, phonons and plasmons; far-field and near field spectroscopies; many body optical physics; topological photonics; among many others. Through these interactions, N2D seeks to provide a setting where unifying concepts can form, new ideas can be inspired, and new frontiers in theoretical and experimental research on 2D materials nanophotonics can emerge.

Invited Speakers
Ritesh Agarwal (University of Pennsylvania, USA)
Pablo Alonso (Universidad de Oviedo, Spain)
Harry Atwater (Caltech, USA)
Ingrid Barcelos (LNLS, Brazil)
Dmitri Basov (University of Columbia, USA)
Joshua Caldwell (University of Vanderbilt, USA)
Monica Craciun (University of Exeter, UK)
Rainer Hillenbrand (Nanogune, Spain)
Frank Koppens (ICFO, Spain)
Stephanie Law (University of Delaware, USA)
Lefteris Lidorikis (University of Ioannina, Greece)
Sang Hyun Oh (University of Minnesota, USA)
Ajit Srivastava (University of Emory, USA)
Miriam Vitello (CNR NANO, Italy)
Valentyn Volkov (MIPT, Russia)
Wang Xiaomu (University of Nanjing, China)

Quantum2021 International Conference (Part of Imaginenano 2021)

November 23-25, 2021
BEC, Bilbao
https://www.quantumconf.eu/2021/about.php

Organizing Committee
Antonio Correia (Phantoms Foundation)
Ricardo Díez Muiño (DIPC)
Pablo Ordejón (ICN2)
Valerio Pruneri (ICFO)
Stephan Roche (ICREA, ICN2)
Daniel Sánchez Portal (CFM-CSIC)

Quantum Science and Technologies have a huge potential to impact established industrial sectors, building new emerging industries and niche segments and creating economic value. The ongoing progress on building quantum computers, together with the push of quantum technologies including secure communication, sensing and quantum simulations are complemented by the vast family of emerging quantum materials (2D materials, topological insulators, Weyl semimetals, twisted (Moiré) van der Waals heterostructures, etc) which offer a revolutionary playground for fundamental science but also already put in perspective novel paradigms and future quantum techs combining ultralow-power with resilient and practical implementation and processing of quantum information.

This 1st edition of the Quantum2021 International Conference, aimed at gathering the various communities engaged in these fields, to foster the incubation of new ideas and collaborations at the forefront of Quantum science.

More than 30 high profile worldwide most influential academia & industry experts in this sector presented speeches in this international event on how Quantum science will change the future of technology and impact positively our daily life. Among speakers confirmed, Prof. Ignacio Cirac, Prof. David DiVincenzo and Prof. Tommaso Calarco (Chair of the Quantum Flagship).

Quantum2021 was a three-day in-person event that was meant to gather the key players of the Quantum Community and related sectors.

Invited Speakers
Ignacio Cirac (Max Planck Institute of Quantum Optics, Germany)
Tommaso Calarco (Forschungszentrum Jülich, Germany)
Andrea Ferrari (Cambridge Graphene Centre, University of Cambridge, UK)
David DiVincenzo (FZ Jülich / RWTH Aachen, Germany)
Hugues de Riedmatten (ICFO, Spain)
Silvano de Franceschi (CEA/UGA, France)
Christopher Bauerle (Neel Institut / CNRS, France)
Prineha Narang (Harvard University, USA)
Karyn Le Hur (Ecole Polytechnique, France)
Felix von Oppen (Freie Universität, Germany)
Alba Cervera Lierta (Barcelona Supercomputing Center, Spain)
Daniel Jirovec (IST Austria)
Henning Schomerus (Lancaster University, UK)
Niels Bultink (Qblox BV, the Netherlands)
Ramiro Sagastizabal (Qilimanjaro, Spain)
Carlos Abellan (Quside, Spain)
Jan Goetz (IQM, Finland)
Roman Orus (DIPC/Multiverse, Spain)
Sebastian Etcheverry (Luxquanta, Spain)
Xavier Waintal (IRIG - CEA Grenoble, France)
Alexandre Jaoui (ICFO, Spain)
Wister Huang (ETH Zurich, Switzerland)
Klaas-Jan Tielrooij (ICN2, Spain)
Gloria Platero Coello (ICMM-CSIC, Spain)

Higher Education

Advanced School on Quantum Transport Using SIESTA

May 17-20, 2021
Online
https://www.cecam.org/workshop-details/4/

Organizing Committee
Simona Achilli (University of Milan)
Mads Brandbyge (Technical University of Denmark)
Thomas Frederiksen (DIPC, Ikerbasque)
Pablo Ordejon (Institut Català de Nanociéncia i Nanotecnologia - ICN2)
Nick Papior (Technical University of Denmark)
Zeila Zanolli (Utrecht University)

This five-day online school focused on the field of theoretical condensed matter electronic transport exploiting the non-equilibrium Green's function approach. In particular, recent advances in methodology and implementation were presented in the form of lectures and hands-on sessions on hot topics in the field. The participants learned about advanced features of SIESTA [1], calculations of non-equilibrium properties using TranSIESTA/TBtrans [2], and the Python framework SISL [3]. For example, the school lectures covered a recent scheme introducing truly single-junction transport calculations through flexible real-space self-energies [4] and methods to extract tight-binding Hamiltonians from DFT suitable to deal with very large systems [5, 6]. The workshop also hosted an afternoon online poster session, where all participants were invited to present and discuss their various research projects. Despite the challenges of a virtual setting, a survey indicated that the general satisfaction of the participants was very high.

[1] A. Garcia et al, J. Chem. Phys. 152, 204108 (2020)
[2] N. Papior, N. Lorente, T. Frederiksen, A. García, M. Brandbyge, Comp. Phys. Comm., 212, 8 (2017)
[3] https://github.com/zerothi/sisl
[4] N. Papior, G. Calogero, S. Leitherer and M. Brandbyge, arXiv:1905.11113v1.
[5] G. Calogero, N. Papior, P. Bøggild, and M. Brandbyge, J. Phys. Condens. Matter, 30 (2018)
[6] G. Calogero, N. Papior, M. Koleini, M. H. L. Larsen, and M. Brandbyge, Nanoscale, 11, 6153 (2019)

Invited Speakers
Mads Brandbyge (Technical University of Denmark)
Gaetano Calogero (Istituto per la Microelettronica e Microsistemi CNR-IMM, Italy)
Pol Febrer (Institut Català de Nanociéncia i Nanotecnologia – ICN2, Spain)
Ernane De Freitas Martins (Institut Català de Nanociéncia i Nanotecnologia – ICN2, Spain)
Thomas Frederiksen (DIPC, Ikerbasque, Spain)
Petr Khomyakov (Synopsys Inc., Denmark)
Pablo Ordejon (Institut Català de Nanociéncia i Nanotecnologia - ICN2, Spain)
Nick Papior (Technical University of Denmark)
Sofia Sanz (DIPC, Spain)
Nils Wittemeier (Institut Català de Nanociéncia i Nanotecnologia – ICN2, Spain)
Zeila Zanolli (Utrecht University, Netherlands)

Topological Matter School 2021

August 16-27, 2021
Online
http://tms.dipc.org/

Organizing Committee:
Maia G. Vergniory (DIPC, Max Planck)
Reyes Calvo (Universidad de Alicante)
Santiago Blanco (DIPC, Ikerbasque)
Adolfo Grushin (CNRS)
Alexander Altland (University of Cologne)

In this year's edition we focused on twisted bilayer graphene, and higher-order and fragile topological phases, among other contemporary topics. We touched on state-of-the-art experimental and theoretical aspects, that allowed students to grasp nuances of the field and develop their own research lines at the forefront of the field, featuring also a computational hands-on session.

Invited Speakers
Pablo Jarillo-Herrero (MIT, USA)
Andrei Bernevig (Princeton University, USA)
Cecile Reppelin (CNRS, France)
Oskar Vafek (Florida State University, USA)
David Goldhaber-Gordon(Stanford University, USA)
Claudia Felser (MPI-CPFS, Germany)
Rebeca Ribeiro-Palau (CNRS, France)
Cristiane Morais-Smith (University of Utrecht, The Netherlands)
Anton Akhmerov (TU Delft, The Netherlands)
Titus Neupert (University of Zurich, Switzerland)
Jennifer Cano (Stony Brook University / Flatiron Institute, USA)
Tim Kaxiras (Harvard University, USA)
Sami Mitra (PRL, USA)

Introduction and Applications to Molecular Dynamics

October 6, 2021
DIPC, Donostia/San Sebastián
http://dipc.ehu.eus/dipc-courses/introduction-and-applications-to-molecular-dynamics

Prof. Fernando Álvarez González (CSIC-UPV/EHU)

Introduction to the general and broad topic of the computation of the collective properties of a many-particle system by solving the individual classical dynamics of each particle in interaction with the other particles. This field of molecular dynamics is a thriving field that have seen very interesting applications in the topics of soft matter such as biophysics and polymer physics as well as in gas dynamics, reactions and catalysis on solids and even in the general simulation of certain aspects of chemical reactions.

4 lectures of 60 minutes each distributed in the following way:
- A general overview of elements in molecular dynamics simulations.
- Synergetics of neutron scattering techniques and fully atomistic molecular dynamics simulations.
- Applications of atomistic molecular dynamics in polymers and soft matter in general:
  - Linear homopolymers.
  - Polymer blends.
  - Graphite oxide layers intercalated by PEO.
  - Fully atomistic molecular dynamics simulations in water.

Due to Covid-19 restrictions, the lectures took on a hybrid format with in-person attendees as well as an on-line zoom link. The number of in-person attendees was restricted to 34 while it was possible to follow the lectures through the DIPC zoom.

Violence in the Workplace: Moral Harassment or Mobbing, Sexist and Sexual Harassment, by Sexual Orientation or Gender Expression

January 13, 2021
Online

Aitziber Buñuelos and Eraikiz Kolektiboa

DIPC launched its first Equality Plan in 2020 with strategic work areas including the implementation of a protocol for prevention and the care for victims of sexual and gender-based harassment. In 2021, as part of this important endeavor, we organized a session addressed to the community which concluded with more integral training for the counsellors in charge of receiving cases.

These sessions helped provide insight into the phenomena of violence and mobbing or moral harassment in the work place. This type of training promotes the awareness of different scenarios and explains the consequences for the victims. It also helps to identify resources and tools for prevention, detection and intervention if necessary.

Stress Management Course

February 3, 4, 2021
CFM auditorium, Donostia/San Sebastián

Sofia Facal and Manuela Bercioux
Skills for Science and Industry

Stress is a normal physical reaction and can be positive in short bursts, but over long periods of increased stress exposure lead to a decrease in personal well being and work efficiency. A worldwide PhD survey done by Nature in 2019 has reported a high level of stress connected problems within PhD students. This has put the focus on a problem that is affecting many researchers. The Covid-19 pandemic has further intensified the problem, highlighting the need to develop a program to give practical tools to prevent and manage stressful situations.

This course was conducted by Skills4Science and it was structured in 2 sessions.

Session 1
- What is stress? Definition and types of stress
- Stress and how it affects our health: short term and long term effects
- Responding vs. reacting to Stress
- Recognizing personal stress signals
- Handling stress- practical tools

Session 2
- Stress and how it affects our work
- Handling stress at the workplace
- Prevention and healthy habits
- Practical tools: avoiding procrastination, mindfulness

Media Training Course

May 6, 2021
DIPC, Donostia/San Sebastián

Valentinga Rodriguez

The workshop helped our researchers improve their communication abilities in the context of media interviews. In the course, the participants learned how and why is that some scientific stories become a piece of important news. This helped the attendants to identify personal strategies and abilities that will let them communicate their scientific work in a more effective way in media interviews.

This course was conducted by Valentina Rodriguez, a science communication professional with extensive experience in science journalism and astronomy outreach for international observatories, and it was taught in a morning and afternoon 3 interactive and practical sessions, including a feedback session afterwards.

Transformative Leadership Course

September 13-15, 2021
CFM auditorium and DIPC, Donostia/San Sebastián

Sofia Facal and Manuela Bercioux
Skills for Science and Industry

In this workshop, we explored transformational leadership skills in research and academia. In contrast to traditional leadership styles, transformational leadership is focused on encouraging, inspiring, and motivating colleagues and young researchers to innovate and create change, take responsibility and reach performance beyond expectations.

The value of developing leadership skills is often only recognized when people reach senior positions and manage teams. However, providing leadership education can be a way to extend a science graduates' outlook, capacity, and employability. It can provide a pathway for building self-awareness, self-efficacy, interpersonal skills, resilience, and adaptability, all transferable skills employers seek.

The content of the workshop included:
- What is leadership?
- Transformational leadership theory
- Traits of effective leaders
- Individual leadership styles
- Leaders and their group - group roles and dynamics
- How to handle conflicts
- How to encourage, inspire and motivate your group

Special lecture “Advice to a Young Scientist”

December 1-2, 2021
DIPC, Donostia/San Sebastián

Pedro Miguel Echenique
President of DIPC

Pedro Miguel Echenique, President of DIPC, offered his well known talk “Consejos a un@ joven científc@”, especially aimed at young researchers, in 2 morning sessions on consecutive days.

In his talk, professor Echenique reflects on the formative stages of the research career. The talk was of high interest to the PhD students from our wide research community and was attended by around 200 students, both in-person and virtually.

Theses

Functional materials synthesis by surface-supported chemistry under vacuum.
Mohammed Sabri Gamal Mohammed
25/01/2021
Supervisor: Dimas Garcia de Oteyza Felderman

Theory of spin-orbit interactions in electronic transport and light scattering at the mesoscale.
Cristina Sanz Fernández
03/02/2021
Supervisors: Sebastián Bergeret and Juan José Sáenz Gutierrez

Organic conjugated diradicals and polyradicals: electronic structure and photophysical processes.
Maria Eugenia Sandoval Salinas
15/02/2021
Supervisor: David Casanova

Computational study of aromaticity in porphyrinoid systems and photosensitizers from chemical bonding descriptors.
Irene Casademont Reig
23/06/2021
Supervisor: Eduard Matito Casas

Light scattering from high refractive index nanostructures.
Jorge Olmos Trigo
26/11/2021
Supervisor: Nuno de Sousa and Juan Jose Sáenz Gutierrez

Topological materials from a symmetry perspective.
Iñigo Robredo Magro
10/12/2021
Supervisors: Aitor Bergara Jauregi and Maia García Vergniory

Generation of laser driven shocks and their use to study simple compounds at high pressure.
Donaldi Mancelli
15/12/2021
Supervisor: Ion Errea Lope

Density functional theory for steady-state thermoelectric transport with applications to strongly correlated systems.
Nahual Sobrino Coll
15/12/2021
Supervisors: Stephan Kurth and Roberto D’Agosta

UPV/EHU Research Master's in Nanoscience

DIPC, along with CIC nanoGUNE, collaborates in the official master program in nanoscience organized by the Materials Physics Department of the University of the Basque Country (UPV/EHU) and the Materials Physics Center (CFM-CSIC-UPV/EHU).

The Research Master's in Nanoscience has been offered since 2007 with now 163 students having obtained their Master's degree. Almost 30% of our graduates are international students from four continents (Europe, America, Africa and Asia).

Researchers at DIPC participate in this program in various ways and from different perspectives by developing curriculums, giving lectures, acting as counselors to some of the students, and providing seminars on issues of special interest to the students.

In addition, DIPC plays a valuable role, providing essential infrastructure and funding, within its means, to help ensure the proper development of the program.

For more information visit: www.ehu.eus/en/web/master/master-nanoscience

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