
dipc2020
Donostia International Physics Center

ON THE COVER TOPOLOGY IN PHYSICS

Topology is a branch of mathematics that studies the geometry of manifolds. In condensed matter physics, topological materials are currently occupying a central role because of their exciting transport properties described by topological invariants. Photoemission-based techniques and first-principles electronic structure calculations can be combined to study the topological invariants of a given system. One of them is the Chern number, which was measured for the first time in a topological chiral material.

The cover shows the experimental Fermi surface of PdGa, as measured in angle-resolved photoemission. Multifold crossing in the band structure of PdGa provides information about the Chern number value in such a system.

NBM Schröter et al., *Science 369*, 179 (2020)

2020

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2020: The power of Science

2020 was a difficult and challenging year worldwide. It will be remembered for a long time as the year in which the COVID-19 pandemic broke out. It was the year in which many of us were confined at home for different timespans and it was the sad year in which some of us lost our relatives or friends.

2020 was also the year in which science was omnipresent in public debate. The pandemic showed the social necessity of building and sustaining a strong scientific system, as well as the benefits of scientific literacy in society. Scientific knowledge helped us to understand the biochemistry of the COVID-19 virus, to simulate and limit the spread of the disease in the population, and to develop new instruments to prevent and treat the infection. COVID-19 vaccines were generated at unprecedented speed. Thanks to the amazingly fast DNA sequencing of the virus, phase-1 vaccine clinical trials were started in just a few months, when the development of a vaccine typically takes 10-15 years. This exceptional achievement was based on the enormous amount of scientific knowledge accumulated in the last decades through fundamental research, as well as on the activation of an international cooperation network that can be qualified as exemplary.

At DIPC, we were (and we still are) affected by the general situation and the mobility restrictions. One of the most noticeable consequences was the suspension of the international visitors program, a distinctive feature of DIPC's activity. Seminars, colloquia, workshops, and outreach activities were either postponed or transformed into online events. What is more, scientific activity is largely based on creativity, on the exchange of ideas, and on the contrast of complementary knowledge. The COVID-19 pandemic hampered the personal interaction and communication between researchers and complicated the completion of several projects. In these difficult times, we appreciated even more the deep trust and strong support that our public and private Patrons have always manifested for DIPC.

In spite of all these hurdles, the scientific activity at DIPC kept an excellent level in quality and quantity. In terms of scientific production, more than 400 scientific publications were published in 2020 and there were more than 20,000 citations to DIPC articles in the same period. DIPC researchers made outstanding contributions to the fields of condensed matter physics, computational chemistry, advanced materials, chemical physics, photonics, photochemistry, polymer physics, biophysics, cosmology, astrophysics, and particle physics, among others. Furthermore, we launched in 2020 DIPC's first 'Gender Equality Plan', with the general goal of improving equality and diversity in our workplace. The intense and successful activity of our center in the last year was only possible thanks to the commitment, effort, and enthusiasm shown by all the scientific, technical, and administrative members of the DIPC community during these difficult times. We indeed appreciate it very much.

Ricardo Díez Muiño, Director of DIPC and **Pedro Miguel Echenique**, President of DIPC since 2000.

The difficult situation created by COVID-19 made us aware, more than ever, of the power of science. We were able to develop efficient tools to confront the public health emergency created by the pandemic. It is likely that other crises arise in the future triggered by still unsuspected threats. We cannot anticipate their nature and thus we cannot be specifically prepared to tackle them. A solid scientific system and a broad spectrum of fundamental knowledge, shared by an international scientific community, would be the only way to design and generate possible solutions. The efficiency in the implementation of these solutions would also depend on the popular acceptance of scientific culture and on the citizens understanding of the scientific evidence. DIPC contributes to all these aspects: we generate excellent science, we sustain international research networks, and we disseminate science in society.

The relevance of the scientific activity as a collective tool for acquiring knowledge is beyond doubt. Science is also the basis of technology, whose impact in economic terms is immeasurable. In an increasingly technical and globalized world, nurturing a powerful research ecosystem is an almost essential requirement for economic development. Last but not least: science is an essential element of culture. Science shapes our perspective of the world, our place in it, and ourselves as human beings. The history of ideas would be totally different without science. Contributing to these three areas; generation of knowledge, economy, and culture, is our objective at DIPC. ■

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, San Sebastian City Council, and 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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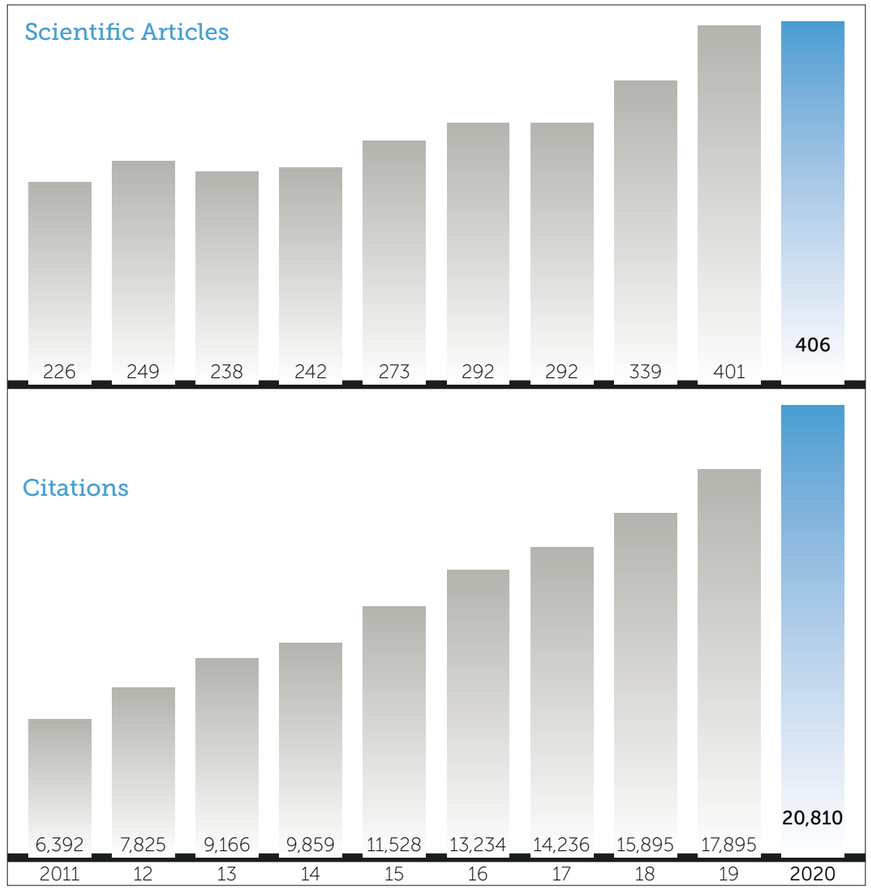
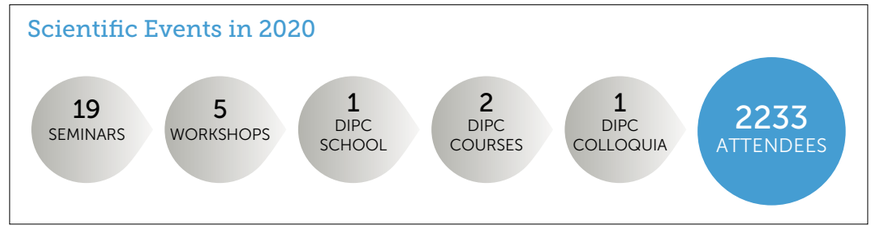
Research Activity at a Glance

In spite of the constraints the COVID-19 pandemic has had on our research activity, DIPC's scientific production and international impact has held up very well. In 2020, **406 scientific articles** were published, slightly more than in 2019 when 401 articles were published. During the last 22 years, the center has published a total of **4,407 ISI publications** and has received more than **156,400 citations**.



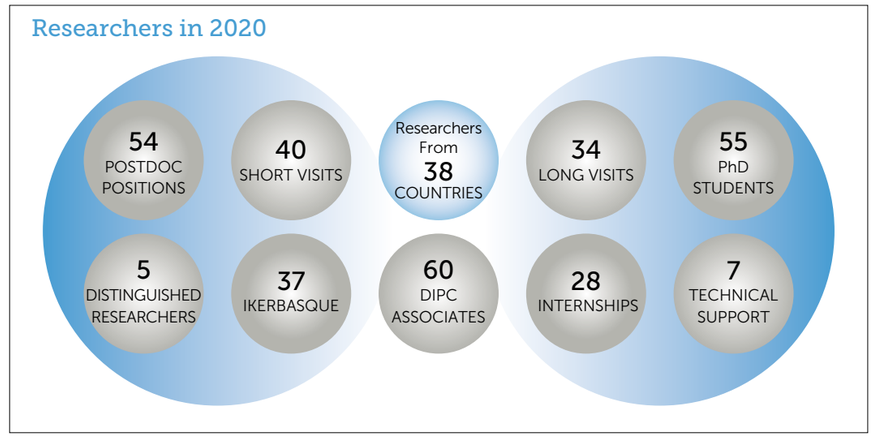
Source Web of Science Core Collection (all years and all indexes, 06/04/2021)



In addition to doing research, DIPC's annual strategic agenda of actions foster exchange with scientists from around the world. Included in the program are Seminars by international experts which cover particular research topics: the DIPC Colloquia which are colloquium-style lectures by outstanding speakers covering all areas of natural sciences, Workshops on specific subjects of interest, and the DIPC Schools and Courses which focus on learning particular skills. Unfortunately, during 2020 part of the programmed events had to be cancelled yet the majority were successfully held online enabling an increase in the number of participants. We enjoyed a more varied attendance from all over the world.

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 to 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 at the Materials Physics Center. Our scientists act as hosts for a generally large number of international visiting researchers and retain the scientific-technical knowledge locally which helps to develop long term DIPC research projects. Among the local host community, there are also Ikerbasque Researchers, who play an important role. Since March 2020, following the recommendations of our public health authorities, DIPC's international visitors program had to be temporarily cancelled.



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.

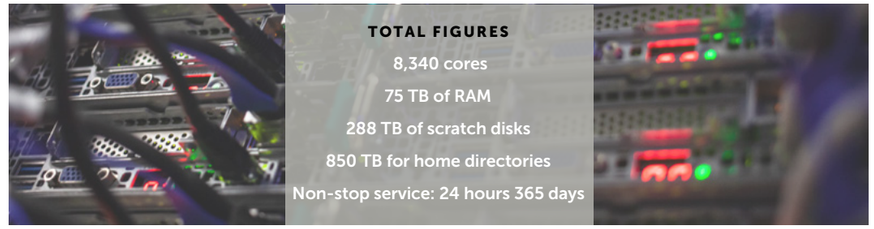
"The variety and power of the computing resources of DIPC, and its constant upgrade, allow the permanent confrontation of a wide range of numerical simulations that put DIPC and other research centers of the Basque Country at the forefront in research"

Txomin Romero Asturiano
Director of the DIPC Supercomputing Center

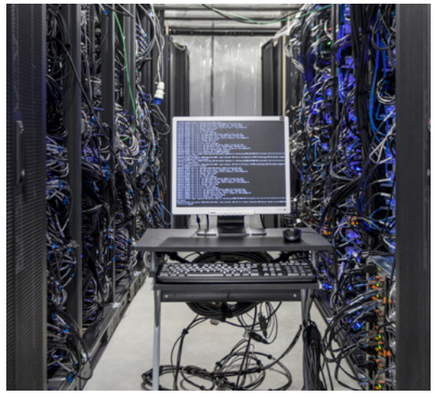
Current computing resources

The Center has three 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 2020, 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 8,000 cores and 70 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.



More than 300 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 or BC3) and Ikerbasque used this computational infrastructure in 2020.



Science Communication

Worth more than ever

2020 was a complicated year in many ways for all of us. DIPC's outreach program was interrupted due to the restrictions imposed during the first surge of COVID-19 in early March. We had to adapt quickly and during confinement we successfully developed an online format. We were able to maintain the majority of our planned activities. Overall, we organized **60 events** with the participation of more than **17,000** in person and virtual attendees. Subsequently there were **54,966** views from various media outlets. We hope that our dedication to the communication of science through our outreach activities continues to stimulate minds and creates some enjoyment during these hard times.

ZIENTZIAKUTXA

Kutxa Fundazioa and DIPC have been organizing a program of dissemination talks aimed at the general public for many years. In 2019, this collaboration materialized in *ZientziaKutxa*, a monthly program combining local and external speakers and a variety of hot scientific topics. In 2020, and after adapting to the pandemic situation, 4 public talks both in person and online were organized with the participation of 680 people and more than 14,000 views in our youtube channel.

Due to the large number of attendees, many people had to follow the talk by Carlos Briones from outside the conference room via live streaming.

14/02/2020
Ruiz Balerdi Hall, Tabakalera
Robótica: retos futuros
Gabe Ibañez Director of Autómata
Concepción Alicia Monje Micharet Universidad Carlos III de Madrid (UC3M)

21/02/2020
Ruiz Balerdi Hall, Tabakalera
El origen de la vida: las raíces del árbol
Carlos Briones Centro de Astrobiologia (CSIC-INTA)

07/05/2020
Online
Neutrinos e imagen médica: la extraña pareja
Paola Ferrario Ikerbasque, DIPC

29/05/2020
Online
Supereroankortasuna, markak hausten!
Ion Errea UPV/EHU, CFM (CSIC – UPV/EHU), DIPC

Paola Ferrario

Ion Errea

CINEMA AND SCIENCE

The Basque Film Archive, DIPC and this year for the first time also the San Sebastian International Film Festival (SSIFF) presented the third edition of the Cinema and Science cycle that took place between January and March 2020 in Tabakalera (Donostia / San Sebastián) and the Bilbao Fine Arts Museum. A total of 10 films were screened with presentations and subsequent discussions led by prestigious scientists. This edition also hosted four science dissemination talks related to the selected movies; two of them in collaboration with Zientziakutxa in San Sebastian and other two in Bilbao thanks to the Chair of Scientific Culture of the University of the Basque Country. Scholar sessions, as well as a special screening took place in Saint Jean de Luz. Unfortunately, one of the gems expected for this edition, the screening of *Frau in Mond* (Fritz Lang, 1929) accompanied by life music, had to be postponed to the next year. Overall, 3,862 people participated in the various screenings in both cities and 859 people attended the public lectures or followed them in streaming.

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

Ágora (Alejandro Amenabar, 2009)
(1) 10/01/2020 (2) 11/01/2020
Physicist **Pedro Miguel Echenique**, UPV/EHU, DIPC

Gilda (Charles Vidor, 1946)
(1) 16/01/2020 (2) 18/01/2020
Chemist **Rosa Errazkin**, Laboratorium Bergara

Gattaca (Adrew Niccol, 1997)
(1) 23/01/2020 (2) 25/01/2020
Jurist and biologist **Leire Escajedo**, UPV/EHU

Proxima (Alice Winocour, 2019)
(1) 04/02/2020 (2) 01/02/2020
Astrophysicist **Silvia Bonoli**, Ikerbasque, DIPC

Her (Spike Jonze, 2013)
(1) 06/02/2020 (2) 08/02/2020
Physicist **Gustavo Ariel Schwartz**, CFM (CSIC-UPV/EHU), DIPC

Autómata (Gabe Ibañez, 2014)
(1) 13/02/2020 (2) 15/02/2020
Engineer **Concepción Alicia Monje**, UC3M
Film director of Autómata **Gabe Ibañez**

The tree of life (Terrence Malick, 2011)
(1) 20/02/2020 (2) 22/02/2020
Chemist **Carlos Briones**, Centro de Astrobiología (CSIC-INTA)

X:The Man with the X-Ray Eyes (Roger Corman, 1963)
(1) 05/03/2020 (2) 07/03/2020
Physicist **Javier Aizpurua**, CFM (CSIC-UPV/EHU)

Awakenings (Penny Marshall, 1990)
(1) 11/07/2020
Neurobiologist **José Ramón Alonso**, Universidad de Salamanca, Instituto de Neurociencias de Castilla y León

Ad Astra (James Gray, 2019)
(1) 22/07/2020
Chemist **Fernando Cossio**, UPV/EHU, Ikerbasque

Public Lectures

29/01/2020
Bidebarrieta Central Library, Bilbao
Energía... ¿oscura?
Marcos Pellejero DIPC

26/02/2020
Bidebarrieta Central Library, Bilbao
Herramientas de luz: de la ciencia ficción a las películas moleculares
Nerea Zabala UPV/EHU, DIPC

Two more public lectures were organized in San Sebastian related to the cinema and science screenings in the framework of Zientziakutxa. **Carlos Briones**, **Concepción Alicia Monje Micharet** and **Gabe Ibañez** participated in those two events.

Scholar sessions

Special morning sessions for students screened "The Day After tomorrow" (Roland Emmerich, 2004) presented by local experts in climatology and served to reflect on climate change and global warming:

11/02/2020 and 18/02/2020
Donostia / San Sebastián
Onintze Salazar Physicist from Euskalmet

11/03/2020
Bilbao
Jon Arrizabalaga Environmental researcher

Special session

21/01/2020
Cinema Le Sélect
Cinema and Science, Saint Jean de Luz GILDA
(Charles Vidor, 1946)
Ricardo Díez Muiño Director, DIPC
Joxean Fernández Director, Basque Film Archive

WOMEN IN SCIENCE

7-14/02/2020

To commemorate the International Day for Women and Girls in Science that is celebrated worldwide on the 11th of February, female scientists, STEM professionals and allies from DIPC, CIC nanoGUNE, CFM Materials Physics Center (UPV/EHU-CSIC), CIC biomaGUNE, Biodonostia, Tecnun-Escuela de Ingenieros, CEIT, Polymat and Elhuyar Foundation have joined forces to present a complete program of activities aimed at all audiences. The objective is to make the activity of women in science visible, to break with the typically male roles attributed to scientific-technical activities, and to encourage the choice of scientific careers among girls and teenagers.

485 people had the opportunity to experience science from a gender perspective in the 12 activities put together thanks to this highly cooperative alliance:

07/02/2020 | CIC nanoGUNE
Zientzia bada nesken kontua Workshop for girls and female teenagers

07/02/2020 | Club Hall, Victoria Eugenia Theatre
Zientzialariak, atzo eta gaur Public lecture

Clara García Astrain CIC biomaGUNE
Edurne González Polymat
Joanna López Biodonostia
Naiara Rodriguez-Florez Tecnun
Sara Barja CFM (CSIC-UPV/EHU)
Silvia Bonoli Ikerbasque, DIPC

08/02/2020 | Ibaeta Campus
Ginkana kanpusean Scientific games for families

For more information visit:
emakumeakzientzian.eus

11/02/2020 | CIC nanoGUNE, CFM/DIPC, CIC biomaGUNE, Polymat and Biodonostia
Ezagutzen al duzu emakume zientzialaririk? Scholar visits of the research centers

13/02/2020 | CFM/DIPC, POLYMAT, CIC BiomaGUNE and Biodonostia
Amona's Power Hands-on science experiments for +55 women

14/02/2020 | Carlos Santamaria Center
Equality in Science: experiences and future Round table

Speakers:
Xana Belastegi Iden Biotechnology
Naëmi Leo CIC nanoGUNE
Concepción Alicia Monje Micharet UC3M
Idoia Otxoa CEIT-Tecnun
Maria Paulis Polymat, UPV/EHU

Moderator:
Itziar Otegui CIC nanoGUNE

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.

Within the Mestizajes program, different activities such as conferences, seminars, presentations or collaborative projects have been carried out. These activities have the collaboration of the San Telmo Museum, Donostia Kultura, Tabakalera and the Vice Rectorate of the Guipúzcoa Campus of the University of the Basque Country.

During 2020, the following activities have been carried out:

CREATIVIUM PROJECT

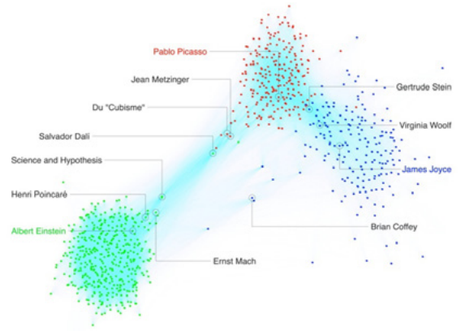
Creativium is a transdisciplinary project that analyses and portrays scientific creativity in an artistic/literary key. The objective of the project is to banish myths and false beliefs and to show that creativity, particularly scientific creativity, is a process that can be developed, encouraged and studied. The project presents the different stages of the creative process (preparation, incubation, illumination and verification) through artistic photographs of scientists in their daily activities accompanied by essays and literary texts about creativity and creative processes. Coordinated by Gustavo Ariel Schwartz, the photographs were taken by Paula Arbide to scientists from DIPC, CFM and Nanogune.

Creativium is a project based on three pillars: a photobook, a photographic exhibition and a website (http://creativium.mestizajes.es). The photographic exhibition was premiered in 2019 in San Sebastián and it is freely available under request for exhibition worldwide.

COMPLEX NETWORKS REVEAL EMERGENT INTERDISCIPLINARY KNOWLEDGE IN WIKIPEDIA

In collaboration with **The CulturePlex Lab** (Canada) we are developing new complex networks based methods in order to approach challenging interdisciplinary problems. These innovative methods allow us mining Wikipedia to unveil implicit interdisciplinary knowledge to map and understand how different disciplines (art, science, literature) are related to and interact with each other. Furthermore, the formalism of complex networks allows us to characterize both individual and collective behaviour of the different elements (people, ideas, works) within each discipline and among them.

For more information visit:
www.mestizajes.es



Interdisciplinary knowledge map. Each dot represents an entry of Wikipedia (related to people, concepts, works) and lines represent links between different elements.

PRIDE IN SCIENCE

CIC nanoGUNE, the Materials Physics Center (CFM, CSIC-UPV/EHU) and DIPC present the space "Orgullo en Ciencia / Harrotasuna Zientzian". Our aim is to give visibility to the LGBTQIA+ collective in science and to actively contribute to demolishing old stereotypes, giving voice and visibility to a plural reality that we want to be a protagonist in the future of science.

In 2019 we joined the international Pride in STEM movement celebrating Pride in Science Day and in 2020, and after establishing a collaboration with PRISMA, we organized our first big event addressed at education where 432 students from 11 schools participated.

18/11/2020 | Online Encounter
Harrotasuna Zientzian / Orgullo en Ciencia

Speakers:
Juani Bermejo-Vega Universidad de Granada
Mari Luz Cádiz Universidad de Granada
Daniel Martínez-Tong CFM (CSIC-UPV/EHU)
Laura Muelas de Ayala UPV/EHU
Marina Peña CFM (CSIC-UPV/EHU)

Moderator:
Javier Armentia Pamplonetario, PRISMA

KIMIKOTEKA

In 2019 the International Year of the Periodic Table was celebrated worldwide to commemorate the 150th anniversary of its creation. That year DIPC conceived KIMIKOTEKA, a singular project to highlight the importance and beauty of the periodic table.

To this end, a collection of wines build up from the chemical elements of the periodic table served to explain the different chemical, physical and biological processes behind the wine. The project was presented in different events at the end of 2019 and beginning of 2020.

02-16/01/2020
Rekondo Jatetxea
17/01 - 14/02/2020
DIPC Headquarters
14/02 - 13/03/2020
Union Artesana
Public exhibition of the KIMIKOTEKA of wines

16/01/2020
Rekondo Jatetxea
Guided wine tasting
Juan J. Iruin Chemist at UPV/EHU
Javier Caneja Sommelier of Rekondo Jatetxea

ON ZIENTZIA

The winners of the 10th edition of the On Zientzia video contest jointly organized by DIPC and Elhuyar Foundation were unveiled at the TV program Teknopolis with an audience of 29,000 people the 13th and 14th of July 2020.

In this edition of On Zientzia, 89 videos participated, among them 51 within the Young Prize Category and 49 videos were in Basque. For the first time, the 54% women participation was higher than men.

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

BEST VIDEO
Técnica científica para leer el futuro: Micropaleontología
María del Pilar Martin Ramos

BEST VIDEO IN BASQUE
Mundu bat ur-tanta baten barnean
Patxi Razkin

YOUNG PRIZE
Ireki begiak zientziaren mundura
Lorea Arbulu
Irati Agirrebengoa

SPECIAL MENTIONS
La CIENCIA del VAPEO | ¿Es VAPEAR mejor que FUMAR?
Amyad Raduan

¿Podrías SOBREVIVIR a una EXPLOSIÓN NUCLEAR?
Amyad Raduan

PEOPLE'S CHOICE PRIZE
Un SESGO cognitivo MUY FRECUENTE en época de COVID-19: Retrospección
Miguel Porvén

SESSIONS FOR KIDS IN THE SAN SEBASTIÁN FILM FESTIVAL

18-26/09/2020
Belodromoa Ikastetxeetan, Schools' premises

The San Sebastian International Film Festival (SSIFF), DIPC and the Basque Film Archive collaborate to link two of the city's hallmarks: its dedication to cinema and its high specialization in science. As a result, in 2019 we initiated a collaboration to offer science-themed cinema during the San Sebastian International Film Festival for kids and students from Gipuzkoa and organized big events at the Velodrome every day during the festival. In 2020 and due to Covid-19, the format was adapted to be celebrated in the classrooms. *Harrapatu Bandera* (Enrique Gato, 2015), an animated film about spatial exploration, was expressly dubbed into Basque and presented by Eneko Axpe, a local scientist currently working for NASA who also answered to the questions rised by the kids. An estimated of 9,241 students from 50 schools have participated in this crowd activity.

DONOSTIA weekINN 2020

DIPC regularly collaborates in the Innovation Week "Donostia WeekINN" that Fomento of San Sebastian organizes every end of October. In 2020, this collaboration was renovated through *Emakumeak Zientzian* with a public lecture that served as tribute to female scientists of the past and present:

28/10/2020 | Online Event
Emakume Zientzialariak Atzo eta Gaur

Lecturers:
Clara García Astrain CIC biomaGUNE
Edurne González Polymat
Joanna López Biodonostia
Naiara Rodriguez-Florez Tecnun
Sara Barja CFM (CSIC-UPV/EHU)
Silvia Bonoli Ikerbasque, DIPC

HIGH SCHOOL VISITS

Since 2014, DIPC and the Materials Physics Center (CSIC-UPV/EHU) organize visits addressed at high school students with the objective of inspiring scientific vocations and showing our daily activities. In 2020, visits had to be interrupted due to the COVID-19 health emergency. Only 5 of the visits planned during the academic year were possible in early 2020 before the start of the pandemic. A total of 175 students participated.

SUPRASPECTIVES

The installation *Suprasprectives*, by the Berlin based artists duo **Quadrature** (Juliane Götz and Sebastian Neitsch) is the first artistic production developed by Medialab Tabakalera, in collaboration with Ars Electronica and DIPC. In the process of creating *Supraspectives*, the artists have gathered the data of 590 (former) spy satellites, whose trajectory the installation follows. A third of them can be considered space trash, as they are obsolete or damaged, but still, they continue overflying us.

The installation calculates the paths of all satellites in real time and speculatively reconstructs the view they are capturing, offering artistically intervened images of what the satellites could be observing. Additionally, a specifically built motorized antenna on the roof connects live with the satellites overflying Tabakalera, transforming their real radio signals into sound.

The production was developed in Medialab Tabakalera, with the collaboration of astrophysicists **Silvia Bonoli** and **Raul Angulo** from the DIPC, the astronomy group of Medialab and the local radio amateur community.

5th ANNIVERSARY OF TABAKALERA

In 2019, the International Centre for Contemporary Culture Tabakalera celebrated its 5th anniversary with a full program of activities open to all citizens around the 11th of September. DIPC participated in two of the programmed events. Along with the Basque Film Archive and the San Sebastian International Film Festival (SSIFF) we organized a special event of Cinema and Science where *HANDIA* was screened. Also, the art and science piece *Supraspectives* was presented in a round table with artists from Quadrature and scientists from DIPC as invited guests.

12/11/2020 | Tabakalera
HANDIA
Directors of the film participated together with guests from the Aranzadi Science Society who have been responsible for the recent discovery of the remains of the giant of Altzo Miguel Joaquín Eleizegui. His life was immortalized in this film that won ten Goya awards in 2018.

Speakers:
Aitor Arregi Film director of Handia
Jon Garaño Film director of Handia
Paco Etxeberria Aranzadi Elkartea
Lourdes Herrasti Aranzadi Elkartea

12/11/2020 | Tabakalera
Art and Science: Quadrature + Silvia Bonoli and Raul Angulo (DIPC)
A conversation about *Supraspectives*

Silvia Bonoli and Raúl Angulo, astrophysicists at DIPC chat with Sebastian Neitsch and Juliane Götz, members of the artistic collective **Quadrature** and authors of the installation *Supraspectives*, about the creative process and the relationship between art and science. The colloquium was led by the cultural director of Tabakalera Clara Montero.

DIPC 2020 The Year in Media

88 newspaper articles | **12** television appearances

Equality at DIPC

Our first Gender Equality Plan (GEP) is the result of a collective process in which staff members representing DIPC's different working areas have been involved through the guidance of external specialized advice. This commission has been in charge of analyzing the current situation of our institution in terms of gender equality and of proposing and designing a series of actions to promote greater equality in our environment.

After an internal poll to the staff, personal interviews and an integral analysis of the functioning and situation of our institution in terms of gender equality, the diagnosis carried out in 2019 concluded that DIPC is a highly masculinized workforce (73.5% men and 26.5% women at the moment), presenting both vertical and horizontal segregation, with women lacking at top management positions. A need to promote balanced panels, talks and congresses was pointed out, as well as, the existence of no specific measures for work-life balance support.

Taking into account the main outcomes or conclusions we reached, the Committee has worked to establish the main objectives and corresponding actions to design DIPC's First Equality Plan that was launched in 2020 and will last four years. This GEP is structured in four main key areas that represent the main challenges identified:

- Organizational culture
- A diverse workforce
- Sexual harassment at the working environment
- Work-life balance

Each key area has its own strategic objectives, and a number of actions to achieve it.

Nevertheless, DIPC has already taken some actions during the last years to work towards gender equality and diversity in science. 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. Besides, we participate since 2019 in the organization of Pride in STEM Day (November 18th). In collaboration with the Gipuzkoa Provincial Council, a specific research grant for excellent female scientists has been created and also a scholarship for female African scientists in the framework of Women for Africa initiative. In 2020 we joined the APS Inclusion, Diversity, and Equity Alliance (APS-IDEA) promoted by the American Physical Society, a community of transformation integrated by 97 prestigious institutions from all over the world.

This is just the beginning. We will keep working to make science fairer and better overall in the following years.

Personnel Segregated by Sex

	Staff Total	Men	Women
Direction & Management			
Management	2	0%	100%
Direction positions	4	0%	100%
Total	6	33.3%	66.7%
Scientific			
Pre-doc	46	23.9%	76.1%
Post-doc	37	24.3%	75.7%
Seniors	3	33.3%	66.7%
Ikerbasque Research Fellow	6	33.3%	66.7%
Ikerbasque Research Associate	10	20%	80%
Ikerbasque Research Professor	10	10%	90%
Laboratory Technicians	4	50%	50%
Total	116	24.1%	75.9%
Technical & Administrative			
Administrative Staff	8	87.5%	12.5%
IT Personnel	7	42.9%	57.1%
Outreach Personnel	2	100%	0%
Total	17	70.6%	29.4%
TOTAL	**139**	30%	70%

DIPC's staff is integrated by 139 researchers and professionals from different domains. Women represent the 30% of the total, while being the 24.1% of the scientific personnel.

*Data as of 23/03/2021

Associates and Visiting Researchers

Our scientific community also includes 59 associate researchers from other institutions, 25% of whom are women, as well as, the contribution of over 200 world-class scientists from top research institutions that every year visit our center.

	Staff Total	Men	Women
Strategic Level			
Associates	59	25.4%	74.6%
Visiting Researchers (2019)*	215	17.7%	82.3%

*Data from 2019 as no representative ones were collected in 2020 due to COVID-19

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Flavin bioorthogonal photocatalysis toward platinum substrates

Gurruchaga-Pereda J, Martinez-Martinez V, Rezabal E, Lopez X, Garino C, Mancin F, Cortajarena AL, and Salassa L
ACS Catalysis 10, 187–196 (2020)

A catalyst is a substance that increases the rate of a chemical reaction without itself undergoing any permanent chemical change. As the catalyst itself takes part in the reaction it may undergo a physical change. Metal complexes are typically regarded as catalysts that convert organic substrates into more valuable compounds; however, to date, catalytic transformations of metal complexes are practically unknown and represent a complete new way of thinking in catalysis. Their development can expand the scope of bioorthogonal chemical reactions to inorganic substances and metal-based prodrugs, fostering the creation of new inorganic chemistry toolkits for biology and medicine.

Bioorthogonality, a term coined by Carolyn R. Bertozzi in 2003, refers to any chemical reaction that can occur inside of living systems without interfering with native biochemical processes. Hence, catalytic turnover can boost the efficiency of bioorthogonal chemical reactions, unveiling new strategies for prodrug activation and uncaging of molecular probes.

In 2017, a team of researchers reported a new type of light-driven reaction in which the exogenous biological molecule riboflavin (Rf) functions as a bioorthogonal photocatalyst and a metal complex acts as an unconventional substrate. This unusual catalyst/substrate pair relies on the photoredox properties of Rf to enable the selective activation of a Pt(IV) prodrug of cisplatin with exceptionally low doses of blue light and induce apoptotic death in PC-3 human prostate cancer cells. Unlike in classic organometallic catalysis, where metals act as catalysts, in this reaction, the metal complex is an unconventional substrate, and the biocompatible riboflavin acts as catalyst.

Apart from these pioneering studies on flavins, the enantioselective synthesis of $[Ru(bpy)_3]^{2+}$ via organocatalysis, and the recent aromatic amination of cyclometalated Ru(II) and Rh(III) octahedral complexes are the three only examples known to date of catalytic reactions that use metal complexes as substrates. This uncharted territory may offer intriguing opportunities to expand synthetic inorganic chemistry and foster new catalysis-based applications for coordination and organometallic compounds.

In order to be able to explore these opportunities it is important to understand how these reactions occur. Now, a new study provides a detailed mechanism through which flavins (photo)catalyze the activation of Pt(IV) complexes.

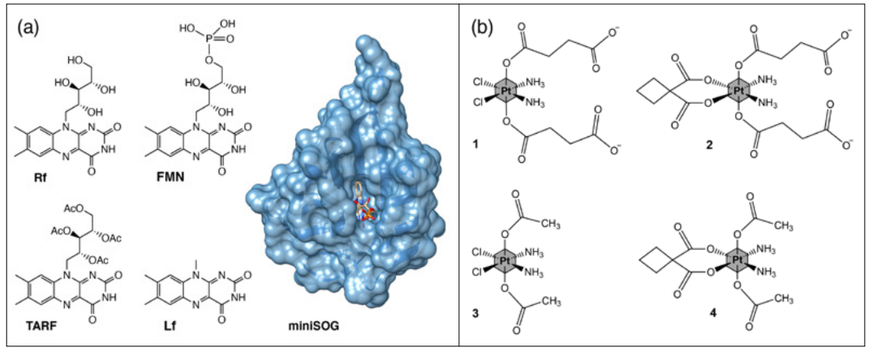


Figure 1. Structures of (a) catalysts and (b) substrates employed in this work. Catalysts: riboflavin (Rf), riboflavin-5′-phosphate (FMN), 2′,3′,4′,5′-tetraacetylriboflavin (TARF), lumiflavin (Lf), mini Singlet Oxygen Generator (miniSOG). Substrates: cis,cis,trans-$[Pt(NH_3)_2(Cl_2)(O_2CCH_2CH_2CO_2)_2]^{2-}$ (1), cis,cis,trans-$[Pt(NH_3)_2(O_4C_6H_6)(O_2CCH_2CH_2CO_2)_2]^{2-}$ (2), cis,cis,trans-$[Pt(NH_3)_2(Cl_2)(O_2CCH_3)_2]$ (3), cis,cis,trans-$[Pt(NH_3)_2(O_4C_6H_6)(O_2CCH_3)_2]$ (4).

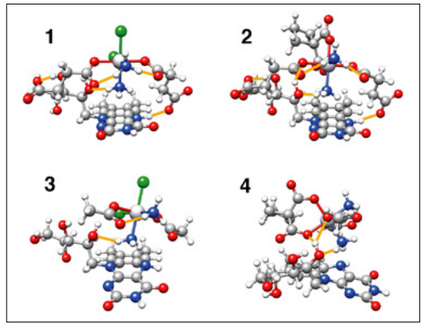


Figure 2. DFT-optimized (pbe0/def2-SVP) structures of adducts between 1–4 and RfH– (H-bond contacts highlighted with orange lines).

Flavins as selective photocatalysts for the activation of Pt-based prodrugs

The researchers use four different free flavins (Figure 1), namely, riboflavin (Rf), flavin mononucleotide (FMN), tetra-O-acetyl riboflavin (TARF) and lumiflavin (Lf), and the flavoprotein miniSOG (mini Singlet Oxygen Generator), together with a panel of Pt(IV) substrates conveniently selected. NMR, steady-state, and time-resolved optical spectroscopy are the experimental techniques employed together with density functional theory calculations (DFT).

They find that the activation via reduction of the Pt(IV) complexes may be influenced by H-bonding interactions between the flavin catalyst and the metal substrate and DFT confirms that both the isoalloxazine and ribityl moieties of the flavins determine the catalytic efficiency of the process (Figure 2).

These findings about the redox chemistry of flavins toward transition metals may have potential implications in the biochemistry and in the cell homeostasis metals other than platinum. For example, flavoenzymes such as mercuric reductase regulates Hg resistance in several organisms by promoting the conversion of highly toxic Hg(II) species to less dangerous Hg(0).

DIPC HIGHLIGHT 2020

Multiscale analysis of phase transformations in self-assembled layers of 4,4 ‘-biphenyl dicarboxylic acid on the Ag(001) surface

Prochazka P, Gosalvez MA, Kormos L, de la Torre B, Gallardo A, Alberdi-Rodriguez J, Chutora T, Makoveev AO, Shahsavar A, Arnau A, Jelinek P, and Cechal J
ACS Nano 14, 7269–7279 (2020)

Understanding the processes that drive self-selection of components into growing phases and their kinetics is of utmost importance in the fabrication of supramolecular nanostructures with defined properties.

A detailed understanding of two-dimensional phase transformations taking place at surfaces requires the use of multiscale analysis involving multiple methods for the characterization of various processes taking place at different time and length scales. Understanding the nucleation and growth kinetics of self-assembled monolayer phases is of special interest, as this type of thin films is used in the construction of devices. However, large scale models of the self-assembly kinetics near thermodynamic equilibrium are still in their infancy. In this work, we explore the use of kinetic Monte Carlo simulations to gain deeper insight. In comparison to molecular dynamics, KMC allows focusing on the simulation of rare events, as opposed to the thermal motion of the atoms around their equilibrium positions, thus, enabling faster calculations.

The thermally-activated removal of a hydrogen atom from the periphery of a molecule (deprotonation) leads to an abrupt change in the chemical nature of the molecule and, consequently, a modification in the intermolecular bonding. This triggers a phase transformation (see Figure 1) from an initial two-dimensional molecular phase α in dynamic equilibrium with the two-dimensional gas of non-deprotonated molecules into a secondary phase β in equilibrium with the corresponding 2D gas of deprotonated molecules (see Figure 2). The overall 2D gas plays an indispensable role in the phase transformation, mediating mass transport between the individual islands and hosting the actual deprotonation reaction from non-deprotonated to deprotonated molecules. Most interestingly, the phase transformation shows a rich variety of phenomena, including Ostwald ripening of the α phase prior to the transformation, burst nucleation of the β phase, remote dissolution of the α phase islands in the vicinity of stable β phase islands and a structural change from disorder to order. These phenomena are well explained by the proposed general growth–conversion–growth (GCG) model (see Figure 2), which is validated by our kinetic Monte Carlo simulations. In the experiments, we consider the phase transformation that takes place on a Ag(001) metal surface induced by the deprotonation of 4,4’ biphenyl dicarboxylic acid (BDA).

The combination of mesoscale information provided by low energy electron microscopy (LEEM) with atomic scale imaging by scanning probe microscopy is essential to unambiguously relate the distinct contrast in LEEM images and the complex diffraction patterns with the particular molecular arrangements associated with the observed molecular phases. Kinetic Monte Carlo simulations and density functional theory calculations provide a qualitative explanation of the underlying physical phenomena. Our findings demonstrate the spatial and temporal evolution of surface phases during their transformation, enabling to assess the key principles and the kinetics of the transformation. Furthermore, the methods used can be considered of general validity.

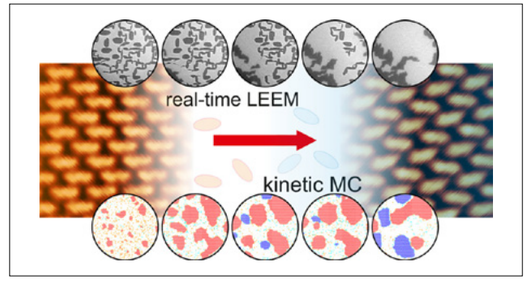


Figure 1. During slow annealing from room temperature upwards, the α → β phase transformation is observed when the temperature becomes 341 K. The upper circles show an image sequence of this transformation, as measured by LEEM in bright field mode at 1.5 eV. STM images on the left/right sides display the molecular arrangement for the α and β phases, respectively. The lower circles show a simulated phase transformation based on the proposed GCG model.

The observed phase transformations are well described by the proposed general growth-conversion-growth model

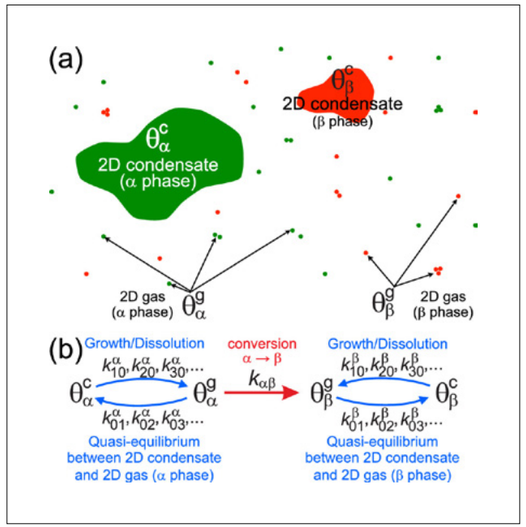


Figure 2. (a) In the GCG model, each molecular phase is associated a ‘2D gas’, referring to the collection of highly mobile aggregates (monomers, dimers, trimers), and a ‘2D condensate’, referring to the rest (nuclei and islands), as shown schematically here for the α and β phases. (b) An abstraction of the proposed GCG model, highlighting the transport between the gas and condensate for each phase, and the rate constants associated with attachment/detachment between the 2D gas and the 2D condensate of each phase (k^{α}_{01}, k^{α}_{02}, ...;k^{α}_{10}, k^{α}_{20}, ...;and k^{β}_{10}, k^{β}_{20}, ...;k^{β}_{01}, k^{β}_{02}, ...;respectively), and the ‘conversion’ reaction with rate constant . In the experiment, the ‘conversion’ reaction consists on the deprotonation of the BDA molecules occurring in the 2D gas of the α phase.

DIPC HIGHLIGHT 2020

Tuning the electronic, magnetic and topological properties of graphene nanoribbons

[1] Probing the magnetism of topological end states in 5-armchair graphene nanoribbons
Lawrence J, Brandimarte P, Berdonces-Layunta A, Mohammed MSG, Grewal A, Leon CC, Sanchez-Portal D, and de Oteyza DG
ACS Nano 14, 4499–4508 (2020)

[2] Band depopulation of graphene nanoribbons induced by chemical gating with amino groups
Li JC, Brandimarte P, Vilas-Varela M, Merino-Diez N, Moreno C, Mugarza A, Mollejo JS, Sanchez-Portal D, de Oteyza DG, Corso M, Garcia-Lekue A, Peña D, and Pascual JI
ACS Nano 14, 1895–1901 (2020)

[3] Magnetism of topological boundary states induced by Boron substitution in graphene nanoribbons
Friedrich N, Brandimarte P, Li JC, Saito S, Yamaguchi S, Pozo I, Peña D, Frederiksen T, Garcia-Lekue A, Sanchez-Portal D, and Pascual JI
Physical Review Letters 125, 146801 (2020)

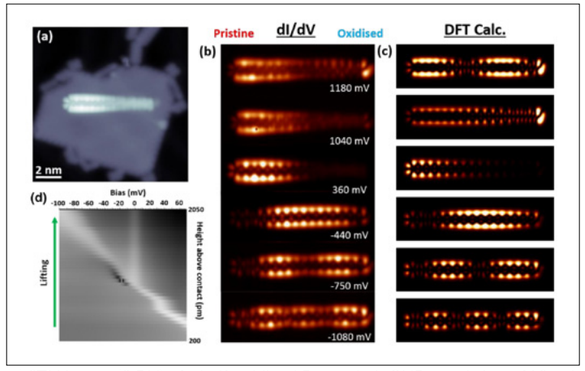
[4] Stabilizing edge fluorination in graphene nanoribbons
Panighel M, Quiroga S, Brandimarte P, Moreno C, Garcia-Lekue A, Vilas-Varela M, Rey D, Sauthier G, Ceballos G, Peña D, and Mugarza A
ACS Nano 14, 11120–11129 (2020)

Graphene nanoribbons (GNRs), are strips of graphene with ultra-thin width (<50 nm). Graphene ribbons, introduced as a theoretical model by Mitsutaka Fujita and coauthors to examine the edge and nanoscale size effect in graphene, have emerged as a promising material for nanoelectronics, as they combine many of the extraordinary properties of graphene with a high tunability of their electronic band structure.

In contrast to graphene, GNRs are frequently semiconducting materials, thus offering excellent perspectives for their utilization as electronic components such as diodes or transistors. The high susceptibility of those properties to minimum changes in the GNR structure means that they can be tuned through the precise control of their atomic building, but also indicates the stringent need for atomic precision in GNR synthesis.

The advent of bottom-up synthesis has opened the path to defect-free GNRs, assembled by on-surface reactions of molecular organic precursors over a metal surface. These strategies rely on the careful design of suitable molecular precursors with specific shape and chemical composition to steer a step-wise reaction on a metal surface, leading to extended and atomically precise GNRs. An ample library of precursors and reaction pathways has been constructed in the last years, incorporating successful examples of precise control over the GNR's width, orientation and edge topology.

This way, ultranarrow graphene nanoribbons (GNRs) with armchair edges and zigzag termini that have five carbon atoms across their width were synthesized on Au(111) [1]. Measurements on the ribbons show well-defined dispersive bands and in-gap states and theoretical calculations indicate that these in-gap states are topological in nature, localized at the zigzag termini of the nanoribbons and, importantly, magnetic.



(a) STM image (0.5 V) of a half-oxidized 5-armchair GNR consisting of 16 unit cells (UC) that has been dragged on top of a 1 ML NaCl island on Au(111) using the STM tip. The pristine end appears brighter due to the presence of an edge state that disappears due to the oxidation in the other end of the ribbon. (b) Constant height dI/dV images of the same ribbon. (c) DFT-calculated gas phase molecular orbitals of a half-oxidised 16-UC 5-aGNR. A generally good agreement is found between the images and the calculations. In particular, the (spatial) shift of the valence band towards the oxidized end is clear in both the experimental results and the calculations, with the opposite effect (i.e. a shift towards the pristine end) seen for the conduction band. (d) 2D conductance map of dI/dV spectra recorded during the lifting of a 5-aGNR over NaCl. Each spectrum was recorded after moving to the next height value (steps of 50 pm). dI/dV intensity is plotted with a logarithmic scale to enhance the visibility of the zero-bias Kondo feature that appears once the edge state crosses the Fermi level (zero of energy) and becomes occupied, indicating the magnetic polarization of the edge state.

Featured on the cover of *Physical Review Letters*, an STM image of a graphene nanoribbon in which a seven-carbon-atom armchair configuration doped by a pair of boron atoms builds up a net magnetic moment.

Substitutional doping with heteroatoms is shown to be an effective route to embed spin chains in graphene nanoribbons, turning them into basic elements of spintronic devices

However, and since most GNRs are semiconducting, a promising method for tuning their band structure is the electrostatic gating effect induced by doping. Chemical doping of GNRs has been achieved through the modification of the molecular precursors to either incorporate substitutional heteroatoms in the carbon backbone or by adding functional groups at the edges.

Thus, amino (NH_2) functional groups have been attached at the edges of chiral GNRs that lead [2] to an upward shift of the electronic bands, with valence band crossing the Fermi level; inserting a pair of boron atoms in the carbon lattice of graphene nanoribbons (GNRs) can enable [3] a magnetic ground state. Even something so chemically challenging as the edge fluorination of GNRs can be resolved designing carefully [4] the right precursor.

The electron–phonon interaction of low-dimensional and multi-dimensional materials from He atom scattering

Benedek G, Manson JR, and Miret-Artés S
Advanced Materials 32, 2002072 (2020)

The discovery of superconductivity in 2D films dates back over 80 years. Initially, these were 2D metallic films deposited on inert substrates, but in recent times more exotic 2D systems have exhibited superconducting properties, such as the surface of topological insulators or twisted bilayer graphene.

Superconductivity is caused by the interactions between atomic vibrations (phonons) and electrons in a lattice. The interaction strength is determined by the electron-phonon coupling constant. Still, the theoretical explanation of the mechanisms involved in these surfaces and 2D systems is not clear, and even the role of electron correlations versus the electron–phonon interaction is not well understood.

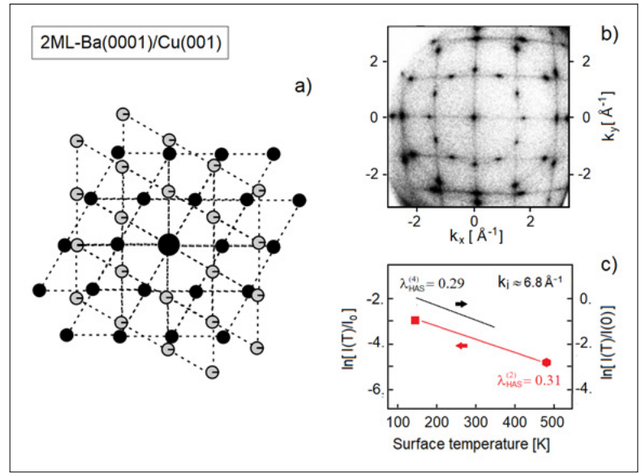
One parameter that has proven to be useful in describing conventional superconductivity in the bulk is the mentioned electron-phonon coupling constant. Now, a team of researchers show that the electron-phonon coupling constant can be measured in the surface region with helium atom scattering experiments, thus enabling a measurement of this useful parameter specific to the 2D surface region.

Very recently, the electron-phonon interaction has been shown to play a relevant role in topological semimetal surfaces such as the quasi-1D charge density wave system Bi(114) and the layered pnictogen chalcogenides. The electron-phonon coupling in these materials for individual phonons, and its average electron-phonon coupling constant, the well-known mass-enhancement factor, can be directly measured with supersonic helium atom scattering (HAS).

A unique feature of low-energy HAS is that the atoms scatter not from the atomic cores of the target surface, but from the rarefied density of electron states whose wave functions extend outward in front of the outermost layer of surface atoms. Thus, the scattered atoms sense the structure and phonon vibrations of the surface atomic cores only through their contributions to the electron density outside (roughly about 3 Å above) the terminal surface layer. Inelastic HAS has been shown to be proportional to the mode-selected components of the electron–phonon coupling constant.

For metal crystal surfaces, inelastic scattering can even detect surface modes for which the largest core displacement amplitudes are located several layers beneath the outermost terminal layer, a property that has been called the quantum sonar effect. With this experimental technique, subsurface phonons were detected on multilayer metallic structures exploring the fairly long range of the electron-phonon interaction, for example, spanning as many as ten atomic layers in Pb films.

Under reasonable approximations, from the thermal attenuation of the diffraction peaks ruled by the so-called Deby-Waller factor, as well as the interaction range through the number of layers, experimental values for some variables can actually be extracted which agree fairly well with previous values for the bulk or obtained from other surface techniques.



(a) A barium bilayer grown on the surface (001) of copper exhibits a dodecagonal quasi-crystalline structure corresponding to the electron diffraction pattern shown in (b). The structure is a superposition of two hexagonal two-dimensional (2D) lattices with a 30° twist, and is the projection of a four-dimensional (4D) honeycomb lattice. The Debye-Waller exponent of the helium atom reflectivity, measured at two different temperatures and the same incident wavevector (c), allows to derive the electron-phonon coupling constant by either treating the bilayer as a 2D (= 0.31) or a 4D (= 0.29) system. The 4D value agrees better with the current value for barium as known in the literature (λ = 0.27).

Helium atom scattering from a conducting surface is shown to provide a direct measurement of the electron-phonon coupling strength for any effective dimension

Here, the team of has focused on the specific role of dimensionality in the electron-phonon mass-enhancement factor as derived from HAS. They are able to extract values for this factor from HAS data for different classes of conducting surfaces characterized by nearly free-electron gases of growing dimensions, from the quasi-1D systems such as W(110):(1 × 1)H and Bi(114), and the quasi-2D layered chalcogenides, to quasicrystalline surfaces such as the dodecagonal 2ML-Ba(0001)/Cu(001) and decagonal d-AlNiCo(00001), which can be regarded as behaving like periodic 4D and 5D materials, respectively.

The analysis of thermal dependence of the Debye–Waller factor measured in the scattering of atoms is based on a theory originally developed for obtaining electron-phonon coupling constant for metal surfaces, adapted now to the more complicated cases of layered chalcogenide semiconductors and systems that can be considered as having different dimensions.

The new analysis shows that, with suitable interpretation of the theory, values of the constant can be obtained from the surfaces of these more complex systems. For all of these systems, the values of the mass-enhancement factor obtained from atom-surface scattering experiments compare favorably with established values for the bulk materials as published in the literature.

Novel van der Waals crystals for phonon polaritons and their characterization

[1] Infrared permittivity of the biaxial van der Waals semiconductor alpha-MoO3 from near- and far-field correlative studies
Alvarez-Perez G, Foland TG, Errea I, Taboada-Gutierrez J, Duan JH, Martin-Sanchez J, Tresguerres-Mata AIF, Matson JR, Bylinkin A, He MZ, Ma WL, Bao QL, Martin JI, Caldwell JD, Nikitin AY, and Alonso-Gonzalez P
Advanced Materials 32, 1908176 (2020)

[2] Broad spectral tuning of ultra-low-loss polaritons in a van der Waals crystal by intercalation
Taboada-Gutierrez J, Alvarez-Perez G, Duan JH, Ma WL, Crowley K, Prieto I, Bylinkin A, Autore M, Volkova H, Kimura K, Kimura T, Berger MH, Li SJ, Bao QL, Gao XPA, Errea I, Nikitin AY, Hillenbrand R, Martin-Sanchez J, and Alonso-Gonzalez P
Nature Materials 19, 964–968 (2020)

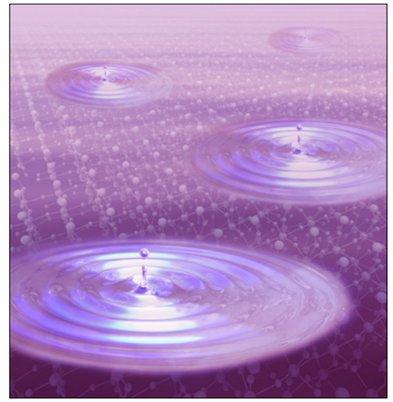
Future information and communication technologies will rely on the manipulation of not only electrons but also of light at the scale of a few nanometers. However, squeezing light to such a small size has been a major goal in nanophotonics for many years. Particularly strong light squeezing can be achieved with polaritons, quasiparticles resulting from the strong coupling of photons with a dipole-carrying excitation, in two-dimensional materials.

One the other hand, even though polaritons can have long lifetimes, they have always been found to equally propagate along all directions (isotropic) both inside the material and along its surfaces, thereby losing energy quite fast, thus limiting their application potential.

Various types of polaritons can be found in materials consisting of two-dimensional layers bound by weak van der Waals forces, the so-called van der Waals materials. In recent years, phonon polaritons – atomic lattice vibrations coupled to electromagnetic waves – with extraordinary properties have been discovered in polar van der Waals crystal slabs. Two examples are dielectric hexagonal boron nitride (h-BN), where phonon polaritons propagation manifests narrow rays leading to hyper-lensing effects, or the semiconductor α-phase molybdenum trioxide (α-MoO_3), which reveals in-plane anisotropic propagation of phonon polaritons with ultra-low losses, offering interesting opportunities for the directional control of light-matter interactions at the nanoscale.

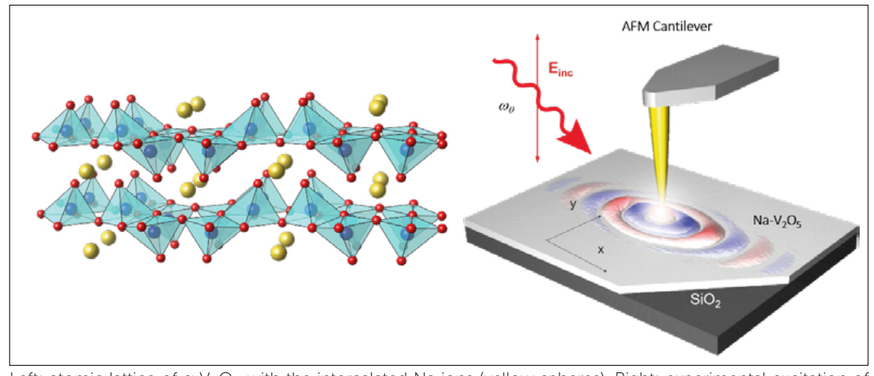
Yet, to accurately predict the infrared response of α-MoO_3 and thus to enable predictive capabilities for advanced optical devices, it is imperative to develop an accurate model for the crystal optical response. The latter would include phonon energies as well as their damping constants, as these parameters are critical for providing insights into how the crystal lattice dictates the optical response of the material.

A team of researchers, including the theoreticians from DIPC – Ion Errea and Alexey Nikitin – have developed an efficient procedure that allows identifying the phonon energies and damping rates on single thick flakes of α-MoO_3 [1]. This sophisticated self-consistent procedure is based on both several experimental techniques, such as ellipsometry and near-field microscopy and theoretical modelling based on density function theory and electromagnetic simulations. The developed innovative approach enables extracting dielectric functions of nanomaterials, where the use of traditional methods is challenging or even not possible.



Novel van der Waals crystal supports hyperbolic polaritons

Artistic illustration of MoO_3 van der Waals crystal supporting anisotropic long-lived phonon polaritons (lattice vibrations coupled to oscillating electromagnetic fields).



Left: atomic lattice of α-V_2O_5 with the intercalated Na ions (yellow spheres). Right: experimental excitation of phonon polaritons in α-V_2O_5 crystal slab by means of near-field optical microscopy. A metallic top is illuminated by an external wave, concentrating the electromagnetic energy into a hot spot below its apex with electromagnetic fields of high momenta. The latter near-fields launch short-wavelength polaritons in the crystal slab. The tip simultaneously plays the role of a probe since it scatters the excited near-fields to the detector.

Despite the extraordinary properties of these phonon polaritons in van der Waals crystals, there is still another important technological drawback for their implementation into nanophotonics technologies, namely the narrow and material-dependent spectral band where they exist (the so-called Reststrahlen band). A broad spectral tuning of a Reststrahlen band in a polar van der Waals material, and consequently of the phonon polaritons supported within it, did not exist.

The same team of scientists showed that chemical intercalation is an efficient route to spectrally tune phonons polaritons in van der Waals crystals, taking as an example the metal oxide α-V_2O_5 [2].

Considering that a large variety of ions and ion contents can be intercalated in layered materials, on-demand spectral response of phonon polaritons in van der Waals materials can be expected, eventually covering the whole mid-infrared range, something critical for the emerging field of phonon polariton photonics.

Enantiospecific response in cross-polarization solid-state nuclear magnetic resonance of optically active MOFs

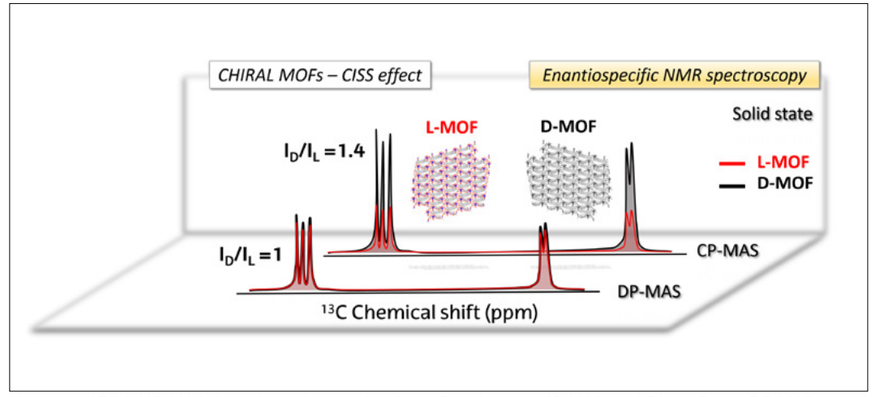
San Sebastian E, Cepeda J, Huizi-Rayo U, Terenzi A, Finkelstein-Shapiro D, Padro D, Santos JI, Matxain JM, Ugalde JM, and Mujica V
Journal of the American Chemical Society 142, 17989–17996 (2020)

Nuclear magnetic resonance (NMR) consists of the resonant absorption of radiation at a photon energy equal to the difference between energy levels of the nuclear-spins split by the action of an external magnetic on non-zero spin nuclei. Since nuclei sense the local electron density determined by the actual electronic structure of the molecule, and this electron density shields the external magnetic field at each individual nucleus, each nucleus will respond to its own distinctly modified effective magnetic field, causing different nuclei to absorb at (slightly) different frequencies (or at slightly different fields for a fixed frequency) depending on the electron density (chemical environment) around each nucleus.

Chiral molecules respond differently to polarized light. This is because chiral molecules can be in one of its two enantiomeric forms. Namely, isomers which are mirror images of each other but have all their internuclear vector distances equal. Thus, enantiomers have identical chemical environments about all their nuclei. Consequently, conventional NMR techniques have been thought to be insensitive to pure samples of pairs of enantiomers. This is because the spin interactions in NMR experiments depend only on the relative vector distances among the active magnetic nuclei, but since they are the same for two enantiomers, measurements of the frequency and the intensity of resonantly absorbed radiation by the magnetically split nuclear-spin states, will yield no difference between enantiomers.

However, a striking departure from this behavior was observed recently by a team of DIPC researchers, who documented an enantiospecific distinct response for a family of chiral aminoacids in a series of NMR magic-angle-spinning cross-polarization (NMR-MAS-CP) experiments, involving the polarization transfer from 1H to 15N nuclei (*ACS Nano* 2018).

These findings challenge firmly established and widely accepted ideas about NMR and enantiospecificity. Consequently, the team understood that additional experiments were needed to build a firmer basis for their hypotheses. So, they engaged in a set of new experiments to lend further support to both, their previous experimental results and the validity of their theoretical framework to account for the physical origin of such a breakthrough observation, which may result vital for future developments in enantiochemistry.



Measured 13C NMR-MAS signal intensities under Cross-Polarization (CP-MAS) and Direct Pulse (DP-MAS) conditions for the D- (black lines) and L-enantiomer (red lines).

Now they report on their results on the NMR 13C signal intensities for both NMR-MAS-CP and NMR-MAS Direct Pulse (NMR-MAS-DP) type experiments carried out on two pairs of optically chiral and enantiopure metal-organic-framework (MOF) molecular ensembles. Results revealed, as predicted by the theory, that under CP conditions 13C NMR signal intensities for the D- and L-enantiomers differ, but under DP conditions they do not, they are not enantiospecific, a conclusive result.

The researchers attributed this striking observation to the onset of electron-spin polarization, accompanying chemical bond electron-density polarization through a chiral center, a secondary mechanism for polarization transfer that is triggered only in the cross-polarization experimental setup. Electron-spin polarization due to the so-called chiral-induced spin selectivity (CISS) effect, creates an enantioselective response, analogous to the one involved in molecular recognition and enantiospecific separation with achiral magnetic substrates. This electron-spin polarization influences the molecular magnetic environment, and ultimately leads to the observed asymmetry in the enantiomers' responses.

The theoretical model to account for the connection between the CISS effect and the remarkable enantiospecific response in Cross-Polarization Solid-State NMR-MAS experiments, have spurred considerable interest and discussion, as reflected in a recent editorial statement on the issue recently appeared on the *Journal of the American Chemical Society* (JACS 2021). Nonetheless, the consistency of these results provides confidence and support to continue the exploration of this ground-breaking research and the implications of these results in the context of spin-specific electron-transfer phenomena at interfaces, and the use of Dynamic Nuclear Polarization techniques in quantum information and quantum storage applications.

Single-chain nanoparticles: opportunities provided by internal and external confinement

Verde-Sesto E, Arbe A, Moreno AJ, Cangialosi D, Alegria A, Colmenero J, and Pomposo JA
Materials Horizons 7, 2292–2313 (2020)

Single-chain nanoparticles (SCNPs) result from the folding individual synthetic polymer chains by means of multiple intra-chain (reversible or irreversible) bonding interactions. The size of these soft nano-objects can be easily tuned between 3 and 30 nm. Only a rough analogy exists between the process of SCNP formation and the precise, specific folding of a polypeptide chain to its native, functional state (e.g., enzymes). Most SCNPs result in a typical morphology in solution more akin to those displayed by intrinsically disordered proteins (IDPs).

Strategies to induce globule formation in SCNPs were also investigated, most of them based on tuning the hydrophobic/hydrophilic balance of the SCNP precursor. The conformational degrees of freedom in SCNPs are severely restricted, giving rise to notorious local domain formation and, hence, to interesting topological self-confinement effects.

Self-confinement in SCNPs has already been exploited for catalysis, encapsulation, transport and delivery of therapeutic cargos, and sensing, targeting and bioimaging applications, as well as a variety of other advanced applications. Further progress is expected in these fields accompanied by the development of new methods of rigorous sequence control and precise placement of single functional monomer units at multiple positions along the polymer backbone. This development will presumably lead to precise control of the SCNP topology and hence to highly accurate structure–property relationships.

External confinement – as imposed under different geometrical constraints as well as in crowded solutions, in the melt state and on surfaces – is an extra parameter to tune the size, shape, dynamics and, hence, potential functionality/foreseen applications of SCNPs. The unifying vision that results by combining recent experiments, simulations and theory suggests that in addition to the global size and shape, external confinement also affects the local internal structure of SCNPs and their dynamics, which are critical e.g. for catalysis and drug delivery applications. This recent knowledge opens up new avenues to tune the properties and functionality of SCNPs (see Figure).

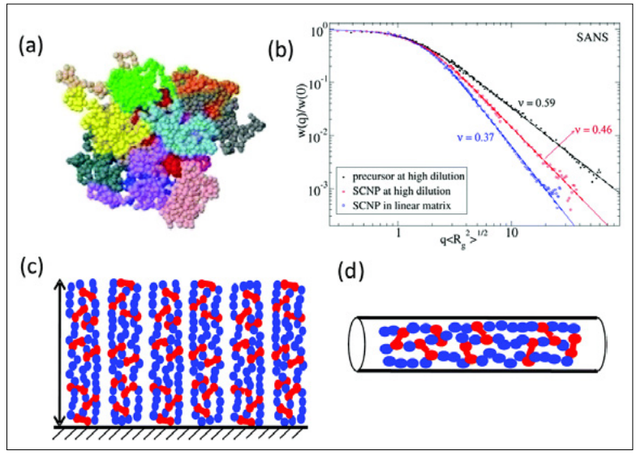


Illustration of external confinement imposed on SCNPs: (a) Crumpled globule morphology of sparse SCNPs (drawn in different colours) in a concentrated solution as revealed by MD simulations. (b) Change in conformation of SCNPs on passing from dilute solution (sparse open conformation, scaling exponent v = 0.46) to all-polymer nanocomposites (crumpled globule conformation, scaling exponent v = 0.37) as determined by SANS experiments. (c) Schematic illustration of arrays of SCNPs on surfaces. (d) Change in conformation of SCNPs in nanopores.

Both self-confinement and external confinement offer a plethora of opportunities to tune the properties of SCNPs for a variety of practical applications

Hence, innovative purification techniques of SCNPs can be envisioned based on their expected behavior during ultrafiltration through nanopores under an elongational flow field. The compact, crumpled globule conformation that sparse SCNPs adopt under crowding, in the melt and in all-polymer nanocomposites often induces significant viscosity reduction effects that could be beneficial for the development of improved all-polymer nanocomposites. Smart responsive surfaces could be foreseen based on a dense array of SCNPs attached to a surface loaded with active substances to be delivered through stimuli-mediated rupture of intra-chain cross-links. Moreover, new topological nanostructures could result by increasing the complexity of the polymer precursors used for SCNP synthesis, their hydrophobic/hydrophilic balance, self-assembly properties, and so on.

DIPC HIGHLIGHT 2020

Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride

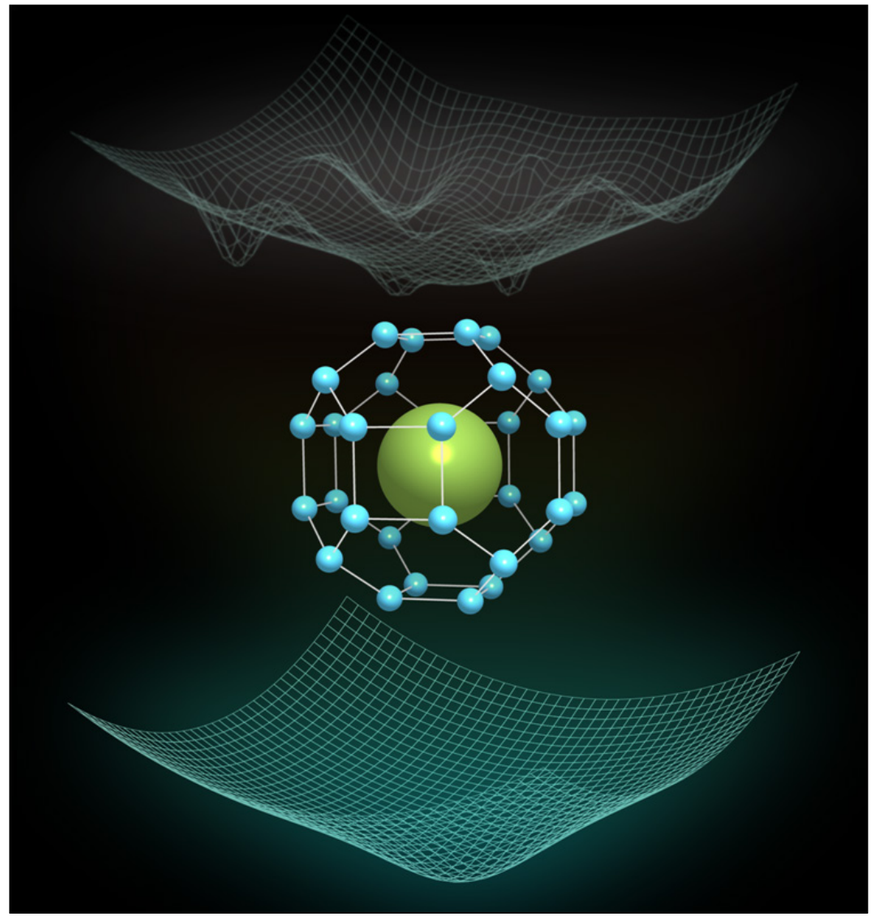
Errea I, Belli F, Monacelli L, Sanna A, Koretsune T, Tadano T, Bianco R, Calandra M, Arita R, Mauri F, and Flores-Livas JA
Nature 578, 66–69 (2020)

Reaching room-temperature superconductivity is one of the biggest dreams in physics. Its discovery would bring a technological revolution by providing electrical transport with no loss, ultra efficient electrical engines or generators, as well as the possibility of creating huge magnetic fields without cooling. The recent discoveries of superconductivity first at 200 kelvin in hydrogen sulfide and later at 250 kelvin in LaH_{10} have spurred attention to these materials, bringing hopes for reaching room temperatures soon. It is now clear that hydrogen-rich compounds can be high-temperature superconductors. At least at high pressures: both discoveries were made above 100 gigapascals, one million times atmospheric pressure.

The 250 kelvin (-23ºC) obtained in LaH_{10}, the usual temperature at which home freezers work, is the hottest temperature for which superconductivity has ever been observed. The possibility of high-temperature superconductivity in LaH_{10}, a superhydride formed by lanthanum and hydrogen, was anticipated by crystal structure predictions back in 2017. These calculations suggested that above 230 gigapascals a highly symmetric LaH_{10} compound (Fm-3m space group), with a hydrogen cage enclosing the lanthanum atoms (see figure), would be formed. It was calculated that this structure would distort at lower pressures, breaking the highly symmetric pattern. However, experiments performed in 2019 were able to synthesize the highly symmetric compound at much lower pressures, from 130 and 220 gigapascals, and to measure superconductivity around 250 kelvin in this pressure range. The crystal structure of the record superconductor, and thus its superconductivity, remained therefore not entirely clear.

Now, this work shows that atomic quantum fluctuations "glue" the symmetric structure of LaH_{10} in all the pressure range in which superconductivity has been observed. In more detail, the calculations show that if atoms are treated as classical particles, that is, as simple points in space, many distortions of the structure tend to lower the energy of the system. This means that the classical energy landscape is very complex, with many minima (see figure), like a highly deformed mattress because many people are standing on it. However, when atoms are treated like quantum objects, which are described with a delocalized wave function, the energy landscape is completely reshaped: only one minimum is evident (see figure), which corresponds to the highly symmetric Fm-3m structure. Somehow, quantum effects get rid of everybody in the mattress but one person, who deforms the mattress only in one single point.

Furthermore, the estimations of the critical temperature using the quantum energy landscape agree satisfactorily with the experimental evidence. This supports further the Fm-3m high-symmetry structure as responsible for the superconducting record.



Crystal structure of the Fm-3m phase of LaH_{10}, where a highly symmetric hydrogen cage encloses the lanthanum atoms. In the top a sketch of the complex classical energy landscape is shown, where many minima are present. On the other hand, in the bottom, the image shows a sketch of the completely reshaped much simpler quantum energy landscape, where only one minimum survives.

This result suggests that superconductivity approaching room temperature may be possible in hydrogen-rich compounds at much lower pressures than previously expected with classical calculations

Fluorescent bicolour sensor for low-background neutrinoless double beta decay experiments

Rivilla I, Aparicio B, Bueno JM, Casanova D, Tonnele C, Freixa Z, Herrero P, Rogero C, Miranda JI, Martinez-Ojeda RM, Monrabal F, Olave B, Schafer T, Artal P, Nygren D, Cossio FP, and Gomez-Cadenas JJ
Nature 583, 48–54 (2020)

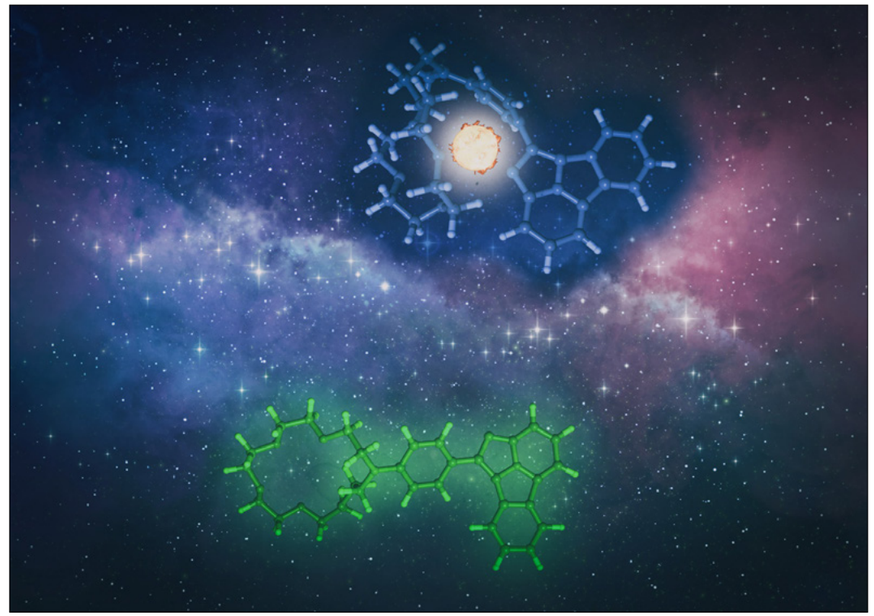
An interdisciplinary team of scientists led by researchers from DIPC, Ikerbasque and UPV/EHU, has demonstrated that it is possible to build an ultra-sensitive sensor based on a new fluorescent molecule able to detect the nuclear decay key to knowing whether or not a neutrino is its own antiparticle.

We know that the Universe is made almost exclusively of matter. However, the Big Bang theory predicts that the early Universe contained the same amount of matter and antimatter particles. This prediction is consistent with the "small Big Bangs" that form in proton collisions at CERN's giant LHC accelerator, where a symmetrical production of particles and antiparticles is always observed. So, where did the antimatter of the early Universe go? A possible mechanism points to the existence of heavy neutrinos that were its own antiparticle, and therefore, could decay into both matter and antimatter. If a second phenomenon occurs, called violation of charge and parity (that is, if the neutrino slightly favors in its decay the production of matter over that of antimatter), then it could have injected an excess of the first over the second. After all the matter and antimatter in the Universe were annihilated (with the exception of this small excess), the result would be a cosmos made only of matter, of the leftovers from the Big Bang.

It is possible to demonstrate that the neutrino is its own antiparticle by observing a rare type of nuclear process called neutrinoless double beta decay (bb0nu), in which concurrently two neutrons (n) of the nucleus are transformed into protons (p) while two electrons (e) are emitted out of the atom. This process can happen in some rare isotopes, such as Xenon-136, which has in its nucleus 54 p and 82 n, in addition to 54 e when is neutral. The NEXT experiment (directed by J.J. Gómez-Cadenas, DIPC and D. Nygren, UTA), located in the underground laboratory of Canfranc (LSC), looks for these decays using high pressure gas chambers.

When a Xe-136 atom undergoes spontaneous bb0nu decay, the result of the process is the production of a doubly charged ion of Barium-136 (Ba^{2+}); with 54 e and a nucleus made of 56 p and 80 n; and two electrons (Xe -> Ba^{2+} + 2e).

So far, the NEXT experiment has focused on observing these two electrons, whose signal is very characteristic of the process. However, the bb0nu process that is meant to be observed is extremely rare and the signal that is expected is of the order of one bb0nu decay per ton of gas and year of exposure. This very weak signal can be completely masked by background noise due to the ubiquitous natural radioactivity. However, if in addition to observing the two electrons, the barium ionized atom is also detected, the background noise can be reduced to zero, since natural radioactivity does not produce this ion. The problem is that observing a single ion of Ba^{2+} in the midst of a large bb0nu detector is technically so challenging that until recently it was considered essentially unfeasible. However, a number of recent works, including this one published in *Nature*, suggest that the feat may be feasible after all.



Artistic representation of the new fluorescent molecule that can shed light on the elusive nature of neutrinos.

A blue spark to shine on the origin of the Universe

The study, led by F.P. Cossio (UPV/EHU, Ikerbasque) and J.J. Gómez-Cadenas (DIPC, Ikerbasque), is based on the feasibility to capture Ba^{2+} with a molecule capable of forming a supramolecular complex with it and to provide a clear signal when this occurs, thus yielding a suitable molecular indicator. The team designed a fluorescent bicolour indicator (FBI) which combines a large intensity enhancement and a dramatic color shift when the molecule captures Ba^{2+}. If an FBI molecule with no barium is illuminated with ultraviolet light, it emits fluorescence in the range of green light, with a narrow emission spectrum of about 550 nm. However, when this molecule captures Ba^{2+}, its emission spectrum shifts towards blue (420 nm). The combination of both features results in a spectacular enhancement of the signal, thus making it very suitable for a future Ba^{2+} detector.

Besides the design and characterization of FBI, the paper offers the first demonstration of the formation of a supramolecular complex in dry medium. This landmark result has been achieved preparing a layer of FBI indicators compressed over a silica pellet and evaporating over such a layer a salt of barium perchlorate.

This work is a significant advance towards building a future "barium-tagging" NEXT experiment to look for noise-free bb0nu events through the identification of the two electrons and the barium atom produced in the reaction. This experiment would have a great potential to find out if the neutrino is its own antiparticle, which could lead to answer fundamental questions about the origin of the Universe.

Advances in topological materials: new magnetic materials and measurements of Chern numbers in semimetals

[1] High-throughput calculations of magnetic topological materials
Xu YF, Elcoro L, Song ZD, Wieder BJ, Vergniory MG, Regnault N, Chen YL, Felser C, and Bernevig BA
Nature 586, 702–707 (2020)

[2] Observation and control of maximal Chern numbers in a chiral topological semimetal
Schroter NBM, Stolz S, Manna K, de Juan F, Vergniory MG, Krieger JA, Pei D, Schmitt T, Dudin P, Kim TK, Cacho C, Bradlyn B, Borrmann H, Schmidt M, Widmer R, Strokov V, and Felser C
Science 369, 179–183 (2020)

Topological materials have special universal properties, which are 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. Topological materials appear ordinary in terms of their bulk bands, but present a special type of conducting states on their surface. These surface states are unique in that they cannot be removed by smooth perturbations, and can never be found in materials that are not topological.

Just as their regular counterparts, topological materials can be broadly classified as either insulators or metals, each with its own interesting properties. In both cases, a topological invariant, an integer number that does not change under perturbations, can be used to pinpoint their topological nature in theory. Experimental proofs of the existence of these numbers are much harder to obtain.

Non-magnetic topological materials have dominated the landscape of topological physics for the past two decades. Research in this field has led to a rapid succession of theoretical and experimental discoveries and, though topological materials were once believed to be rare and esoteric, recent advances in non-magnetic topological materials have found that topological insulators and enforced semimetals are much more prevalent than initially thought.

What about magnetic materials? The short answer being that the breakthroughs in non-magnetic materials have not yet been matched by similar advances in magnetic compounds, due to some big challenges. To start with, there is no theory similar to Topological Quantum Chemistry (TQC) or equivalent methods. If that was not enough, the *ab initio* calculation of magnetic compounds is notoriously inaccurate for complicated magnetic structures beyond ferromagnets. Actually, the number of accurately predicted magnetic topological materials has not reached ten.

The above was true till recently, when a team of researchers performed [1] complete electronic structure calculations, including complete topological phase diagrams, on each of 549 magnetic materials whose magnetic structures have been accurately tabulated (through the careful analysis of neutron-scattering data). Based on these, the researchers were able to predict several novel magnetic topological phases: 130 enforced semimetals and topological insulators in total.

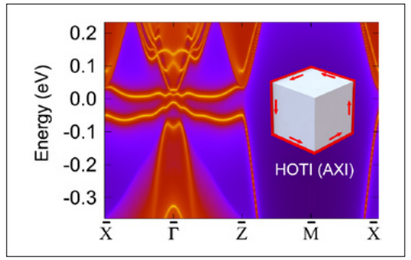


Figure 1. The (001) surface state of the axion insulator NpBi, which has an energy gap of 30 meV. The inset shows a schematic of the chiral hinge states on a cubic sample.

The development of symmetry-based methods to determine topology has been achieved for magnetic materials, allowing the screening of databases to find more than a hundred new materials

The direct detection of surface Fermi arcs in chiral topological semimetals has proved that the maximum topological invariant is achieved in the chiral crystal PdGa

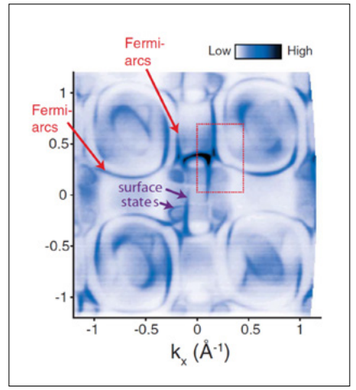


Figure 2. Direct observation of surface Fermi arcs in ARPES reveals the topology of PdGa crystals.

After these great advancements in predictive power, it becomes ever more important to establish experimentally whether a given material is in the predicted topological phase, and to measure its topological invariant.

This notable challenge has recently been tackled in the important case of chiral topological semimetals, where linear band crossings near the Fermi level carry a topological invariant known as the Chern number. This Chern number determines the number of surface states, known as Fermi arcs, that must connect the linear band crossings at the surface. For these types of systems, the largest predicted value of this number is 4, but this had not been observed experimentally.

Scientists have overcome [2] the obstacles that prevented that experimental confirmation by investigating a different chiral topological semimetal candidate from those already tested: the intermetallic compound of palladium and gallium, PdGa. It belongs to space group 198, a family of chiral semimetals —including RhSi, CoSi, AlPt, and PdBiSb— which is expected to display the maximal Chern number of 4.

Using angle-resolved photoelectron spectroscopy (ARPES) and *ab initio* calculations, the researchers can clearly resolve the presence of multifold crossings in the bulk electronic structure of PdGa, as well as four topological Fermi arcs on its surface. This is equivalent to observing experimentally a Chern number 4. Furthermore, the researchers were able to grow chiral crystals with opposite handedness and realized that the sign of the Chern number is reversed by this process, so that surface Fermi arcs propagate with opposite velocities near the nodes.

A Josephson phase battery

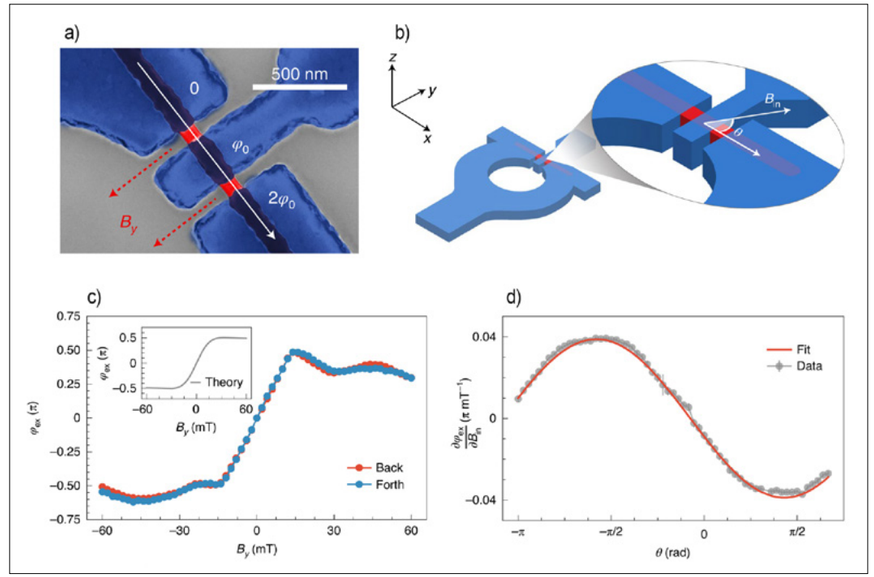
Strambini E, Iorio A, Durante O, Citro R, Sanz-Fernandez C, Guarcello C,
Tokatly IV, Braggio A, Rocci M, Ligato N, Zannier V, Sorba L, Bergeret FS, and Giazotto F
Nature Nanotechnology 15, 656–660 (2020)

Strambini et al. demonstrate a quantum device that provides a persistent phase bias to a superconducting circuit. It consists of a InAs nanowire proximitized by Al superconducting leads. The ferromagnetic polarization of the unpaired-spin states is efficiently converted into a persistent phase bias across the wire. The observed symmetries in the magnetic field confirm the predictions of the theoretical model previously presented by the authors.

A classical battery converts chemical energy into a persistent voltage bias that can power electronic circuits. We denote a phase battery as a quantum device that provides a persistent phase bias to a quantum circuit's wave function. It represents a key element for quantum technologies based on phase coherence. In the present work, the authors demonstrate the first implementation of a phase battery in a hybrid superconducting circuit.

The device is shown in figure (a). It consists of an n-doped InAs nanowire (red) with unpaired-spin surface states, proximitized by Al superconducting leads (blue). The authors found that the ferromagnetic polarization of the unpaired-spin states is efficiently converted into a persistent phase bias φ_0 across the wire, leading to the anomalous Josephson effect. The phase bias can be controlled by an external magnetic field [Figure (b)], achieving a continuous tuning of φ_0 [Figure (c)]. Hence, it is possible to charge and discharge the quantum phase battery. The observed symmetries of the anomalous Josephson effect in the vectorial magnetic field agree with the theoretical predictions done by S. Bergeret and I. Tokatly from DIPC, in a previous work.

These results demonstrate how the combined action of spin-orbit coupling and exchange interaction induces a strong coupling between charge, spin, and superconducting phase, able to break the phase rigidity of the system. This quantum element, providing a controllable and localized phase bias, can find applications in different quantum circuits such as an energy tuner for superconducting flux and hybrid qubits, or a persistent multi-valued phase-shifter for superconducting quantum memories as well as superconducting rectifiers. Moreover, the magnetic control over the superconducting phase opens new avenues for advanced schemes of topological superconducting electronics based on InAs junctions.



(a) Scanning electron microscopy image of the active region of the phase battery composed by the two φ_0-junctions. B_y is the in-plane magnetic field orthogonal to the nanowire. (b) Sketch of the interferometer with the reference axes of the in-plane magnetic field (B_{in}) and the angle θ with respect to the nanowire axis. (c) Dependence of the extrinsic anomalous phase φ_{ex} on B_y. It results in an odd symmetry and non-hysteretic back and forth sweeps (blue and red traces). Inset: the $\varphi_{ex}(B_y)$ dependence obtained from our theoretical model. (d) Plot of $\partial\varphi_{ex}/\partial B_{in}$ versus θ together with a theoretical fit (red curve).

Predictions done by the Mesoscopic Physics group at CFM on spontaneous currents in systems with strong spin-orbit coupling have been experimentally verified in this collaboration

DIPC HIGHLIGHT 2020

Sub-femtosecond electron transport in a nanoscale gap

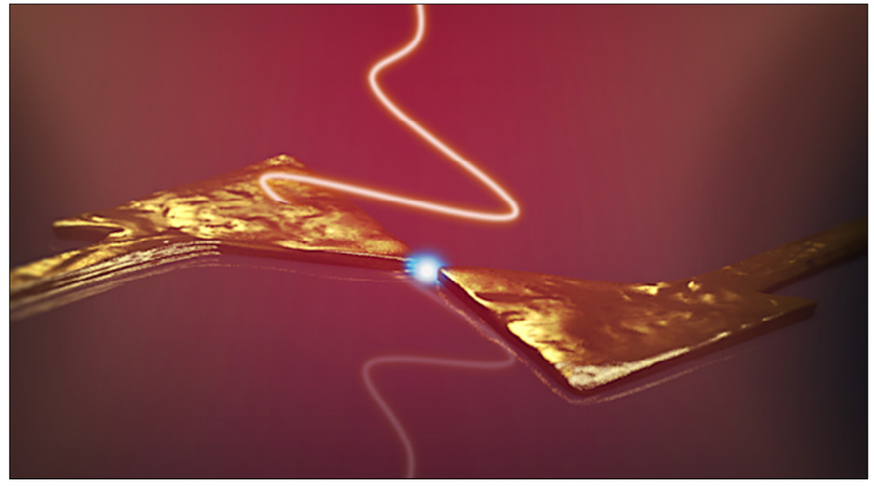
Ludwig M, Aguirregabiria G, Ritzkowsky F, Rybka T, Marinica DC, Aizpurua J, Borisov AG, Leitenstorfer A, and Brida D
Nature Physics 16, 341–345 (2020)

Controlling the movement of electrons in a metal circuit can be achieved by using the carrier envelope phase of ultra-fast laser pulses at optical frequencies. This achievement shows great potential to accelerate data processing speed and could contribute to transforming the computing paradigm of the future, as well as many other applications in optoelectronics.

The technological achievements in electronics have been remarkable over the course of the last decades with a major impact on the society that has firmly evolved towards the digital age. In a simplistic description, the fundamental principle behind the current digital revolution can be related to the ability to open and close an electrical circuit as quickly as possible in order to perform an operation on a sequence of bits. In fact, modern transistors can operate at frequencies below 1 GHz, which corresponds to a billion operations per second. Currently, the most common platform to achieve this result is based on semiconductors, such as silicon, which have reached their optimum performance, and have already started to present objective difficulties in improving the speed required by electronic components. To solve this technological bottleneck, an international collaboration involving researchers from the DIPC and the Material Physics Center (CFM) in San Sebastián, the University of Luxembourg, the University of Konstanz (Germany), and the Institute of Molecular Sciences in Orsay (France) has used laser light to manipulate the electrons in an ultra-fast way. Light has the advantage of oscillating at frequencies several million times faster than those achieved in purely electronic circuits, therefore, controlling a circuit at such (ultrafast) optical frequencies shows enormous potential to change the speed of data processing.

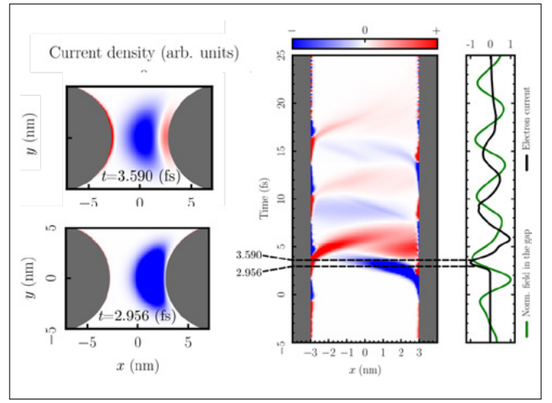
To achieve the manipulation of electronic motion in circuits at optical frequencies might still require many years, however the experiments and theoretical developments carried out by the international team of researchers show that it is possible to use the oscillation of the electric field contained in a pulse of ultra-short laser light to move electrons through a nanoscopic metallic cavity on femtosecond (10-15 s) time scales, creating an otherwise open circuit. The theoretical backup of researchers at DIPC and Orsay have managed to trace the movement of the electrons during those ultra-fast times induced by the laser pulse that controls them. This analysis has allowed for identifying ultrafast burst of electron currents which provide a total net current as a function of the carrier envelope phase of the applied pulse, thus introducing a way to optically control the DC electron current. The results of this work have a fundamental impact on the understanding of how light interacts with matter, especially in a regime of interaction in which it is possible to observe quantum phenomena that occur on scales of space and time that were previously inaccessible.

The impact of these results also affects a wide range of applications in nanotechnology, particularly in optoelectronics, and is a reflection of the ability to manufacture nanodevices formed by highly precise nanostructures capable of manipulating electrons, as well as the development of innovative laser light sources. The level of conceptual compression and monitoring of the movement of the electrons (their dynamics) within a nanodevice serves to design and implement more complex non-linear operations in optoelectronic nano-circuits.



Bowtie nanoantenna (bright areas) forming a nanogap (blue bright spot). An incident single-cycle laser pulse generates ultrafast motion of electrons within the cavity which are able to close the electrical circuit, and thus generate a DC current.

Taming ultrafast electrons with ultrafast light pulses has been achieved



Calculated current density induced in a 6 nm-wide metallic nanocavity induced by an ultrafast optical pulse. Panels to the left show the electron current density (in blue and red) at the cavity at two times. The central panel shows the evolution of the electron current density induced by the pulse along 30 femtoseconds of time. Red stands for positive charge, and blue for negative. The panel to the right shows the normalized field of the pulse at the gap (in green), and the total electron current as a function of time.

The dynamics of ultrafast electron burst in a nanocircuit can be computed and traced

DIPC HIGHLIGHT 2020

Full counting statistics of topological defects after crossing a phase transition

Gomez-Ruiz FJ, Mayo JJ, and del Campo A
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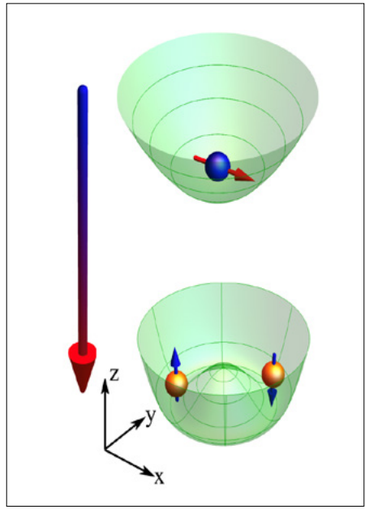
Nonequilibrium phenomena occupy a prominent role at the frontiers of physics. Since its conception in the mid-70s, the Kibble-Zurek mechanism (KZM) has been the paradigmatic framework to describe the dynamics of phase transition, in which symmetry breaking leads to the formation of topological defects (e.g., vortices in a superfluid or kinks in a spin chain). The KZM accounts for the dynamics of a phase transition and was initially developed for a scenario of spontaneous symmetry breaking, illustrated in Figure 1. Its key testable prediction is that the average number of topological defects scales as a universal power law with the quench rate at which the critical point is crossed.

KZM has inspired steadily research over the last three and a half decades since its conception. Progress has been particularly exciting in the last few years pushing the limits of the framework in novel settings including, e.g. ion chains, colloidal monolayers, quantum simulators and quantum computers. And yet, all research to date has predominantly been focused on the characterization of the mean number of defects, overlooking other signatures of universality.

In this work, the authors focus on signatures of universality beyond the mean number of topological defects and show that the full counting statistics of topological defects is actually universal. In particular, they argue that i) the defect number distribution is binomial, ii) all cumulants are proportional to the mean and scale as a universal power law with the quench rate, iii) this power law is fixed by the KZM scaling.

This knowledge allows one to characterize universal features regarding the onset of adiabatic dynamics (probability for no defects) and large deviations of the number of kinks away from the mean value. This prediction is experimentally testable in the wide range of physical platforms in which the KZM has been studied: trapped ion chains, liquid crystals, Bose-Einstein Condensate clouds, colloidal monolayers, to name just a few instances. The authors' findings provide a comprehensive set of predictions that can be subjected to extensive theoretical, numerical and experimental verification and applied to various disciplines and experimental systems.

To date, these predictions have been theoretically explored in trapped ions and holographic superconductors. They have also been experimentally demonstrated in commercially-available quantum annealers, where they provide a benchmark for the performance, e.g., of D-Wave machines.



Knowledge of the kinks statistics bounds errors in Adiabatic Quantum Computing

Figure 1. Critical dynamics. Landau free energy landscape across a continuous phase transition in a U(1) spontaneous symmetry breaking scenario. The quantum critical dynamics induced by crossing the critical point in finite-time is described by the Kibble-Zurek mechanism exploiting the divergence of the relaxation time. Similar ideas have been applied in more complex scenarios without a "clean" critical point.

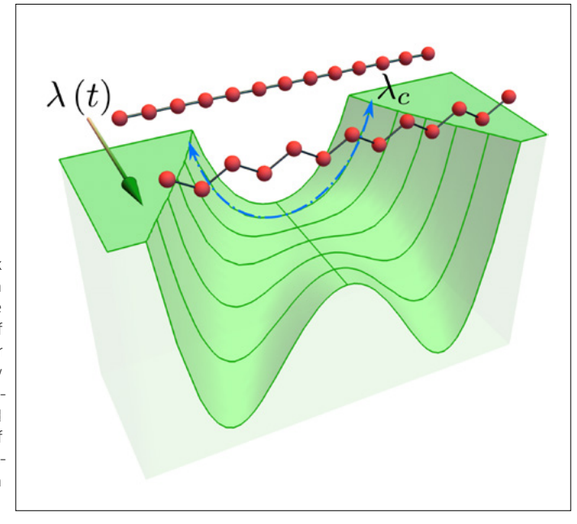


Figure 2. Since the 70's, Kibble-Zurek mechanism has been the paradigm to describe the dynamics of phase transition leading to formation of topological defects. It predicts their mean value as a universal power law with the driving time. This work unveils signatures of universality beyond KZM and shows that the statistics of topological defects, onset of adiabaticity and large deviations away from the mean are all universal.

Kerker conditions upon lossless, absorption, and optical gain regimes

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A nanoantenna with balanced electric and magnetic dipole moments exhibits a directive radiation pattern with zero backscattering. This is known as the first Kerker condition after Kerker, Wang, and Giles, who predicted in 1983 that, under plane wave illumination, magnetic spheres with equal relative permittivity and permeability radiate no light in the backscattering direction. They also concluded that, for certain permittivity and permeability relations for nanospheres, this zero optical light scattering condition happened in the forward direction.

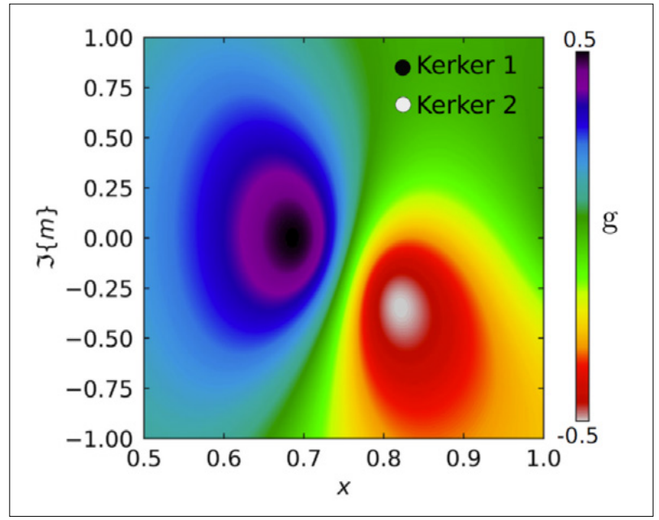
Three decades later, a renewed version of these ideas was proposed for subwavelength dielectric spheres of high refractive index (HRI) materials, reinvigorating the interest on these light scattering conditions. Interestingly, the scattering properties of HRI nanospheres can be fully described by dipolar modes. At the first Kerker condition the electric and magnetic dipolar modes oscillate in phase with equal amplitude. This optical response drives to destructive interference between the scattered fields at the backscattering direction, which is commonly referred to as the zero optical backscattering condition.

This anomalous light scattering condition was first experimentally measured in the limit of small particle in the microwave regime for ceramic spheres and, soon after, in the visible spectral range for HRI Si and GaAs nanospheres.

However, recent results suggest that the concept of small particle is sufficient, but not necessary, to guarantee a dipolar response in the optical scattering of an object. Consequently, the mentioned backscattering anomalies could also be measured on larger dielectric particles.

The absence of backscattered light emerges at the first Kerker condition for dipolar particles regardless of the incoming polarization. On the other hand, for cylindrically symmetric particles, the absence of backscattered light follows from the preservation of electromagnetic helicity. Conservation of helicity has proven crucial in many applications such as enhanced chiral light-matter interactions, or in the spin-orbit interactions of light. Remarkably, it has been reported that from a relatively simple far-field measurement of the electromagnetic helicity at a right angle, the radiation pattern of the dipolar particle is inferable.

Now, a team of researchers analytically demonstrate that either losses or optical gain inhibit the first Kerker condition for homogeneous spheres regardless of the particle's size, incident wavelength, incoming polarization, and multipole order. It follows that dissipating spheres such as dielectric Mie spheres in the visible spectral range and plasmonic particles, such as metal spheres, cannot exhibit the first Kerker condition.



(a) Real (dash-dotted red) and imaginary part (dashed-red) of the refractive index contrast (m) vs the incident wavelength (λ) for a Ge sphere. Maximum of the expected value of the EM helicity in solid blue, ⟨Λ⟩max, for a Ge sphere vs λ under plane wave illumination with σ=+1. (b) Color map of ⟨Λ⟩ vs λ and particle's size (R) for a Ge sphere under plane wave illumination with σ=+1. The visible range is encompassed by a dashed rectangle. As mentioned in the text, in this region helicity conservation is never fulfilled.

> Either losses or optical gain inhibit the emergence of the first Kerker condition of zero backscattering for homogeneous spheres regardless of the particle's size, incident wavelength, incoming polarization, and multipole order

For a germanium (Ge) sphere in the dipolar regime, the team quantifies the gradual drift from the ideal zero optical backscattering condition as the absorption rate is increased. Finally, that optical gain is mandatory to reach the zero forward light scattering condition is demonstrated.

The researchers show that the electromagnetic helicity cannot be preserved after scattering by an arbitrary dielectric sphere in the presence of losses or optical gain. Hence, neither can the zero optical backscattering condition be fulfilled in that scenario.

These results unveil a hidden connection between two symmetries from fundamental principles: energy conservation, mathematically expressed in terms of the optical theorem, and the electromagnetic duality, which is restored at the first Kerker condition. This intriguing link opens new insights into Mie theory.

Fine grained tensor network methods

Schmoll P, Jahromi SS, Hormann M, Schmidt KP, Orus R
Physical Review Letters 124, 200603 (2020)

The concept of vector should be familiar: a quantity for which both magnitude and direction must be stated. This compares with a scalar quantity, where direction is not applicable, like temperature in a precise point. But, what if the magnitude varies with the direction? A vector would be a particular case, with only one direction, but it is possible to think of quantities that have different values for different directions. Welcome to the world of tensors.

You may have heard about tensors in connection to general relativity where they are used to describing spacetime. But tensors have also found their way into the realm of quantum many-body problems through tensor networks. Tensor networks (TN) are mathematical objects which use the knowledge about the amount and structure of entanglement in quantum many-body states in order to reproduce the state accordingly. TN states also show up in other disciplines, such as quantum gravity, artificial intelligence, and even linguistics.

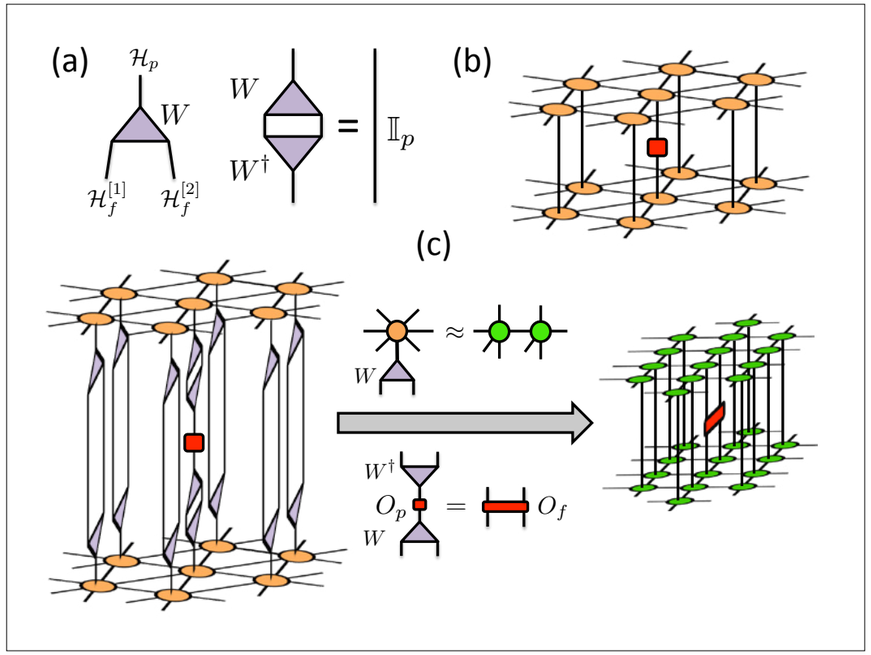
During the past decade there has been a rapid development of tensor network states and numerical methods for simulating strongly correlated quantum many-body systems. These TN methods use Ansätze – educated guesses or additional assumptions made to help solve a problem, and which is later verified to be part of the solution by its results – with remarkable success to simulate quantum lattice systems in different regimes.

Despite being extremely versatile, TNs are not free from limitations, though. The most obvious one is the ability to capture the expected structure of entanglement in the TN Ansatz, i.e., to incorporate the correct scaling of the entanglement entropy. Too much entanglement in the quantum state is a limitation itself.

On top of these limitations, geometric bottlenecks are an additional problem to deal with. A similar one arises for higher-dimensional systems, where high-connectivity lattices are quite usual. This is a serious issue, since such large-connectivity lattices are usually linked to exotic phases of matter such as quantum-spin liquids. In both cases, handling tensors with so many indices, quickly becomes computationally expensive for numerical simulations.

Now, a team of researchers proposes a physically motivated strategy to solve this problem in an efficient and accurate way. The idea is to break down the physical degrees of freedom into "smaller" pieces, i.e., to fine-grain the lattice. This can be done at the expense of introducing a set of fine-graining isometries. Under suitable conditions, then, this fine-graining simplifies the lattice and essentially keeps locality of interactions.

In other words, unlike other proposals of TN methods for high-connectivity lattices, this new approach preserves the correct geometric structure of the system, being better suited in terms of the entanglement structure. The key advantage being that the fine-grained lattice is easily amenable to TN methods.



(a) Isometry W projects the fine-grained Hilbert spaces $\mathcal{H}_f^{[1]}$ and $\mathcal{H}_f^{[2]}$ into the physical space $\mathcal{H}_p$ The isometry verifies $W^\dagger W = \mathbb{I}_p$, with $\mathbb{I}_p$ the identity in the physical space. (b) Expectation value of a one-site operator for a 2d PEPS on a triangular lattice: (c) by introducing resolutions of the identity $W^\dagger W$ at every site, we can rewrite the expectation value in terms of a fine-grained two-site operator and fine-grained PEPS tensors on a 2d square lattice. As such, working with the original operators on the original triangular lattice is equivalent to working with fine-grained operators on the square lattice.

Complex lattices made easy

The simulation of a triangular lattice with projected entangled pair states, for example, would naively imply tensors with six bond indices, if we were to use one tensor per lattice site. Handling tensors with so many indices quickly becomes a computational nightmare. The researchers use the fine-grain approach to compute ground-state properties of some models of the triangular lattice and benchmark the results against those obtained with perturbative continuous unitary transformations and graph projected entangled pair states, showing excellent agreement and also improved performance in several regimes.

This new approach will allow overcoming the computational cost associated to simulating lattices of high connectivity, such as the ones typically found for higher dimensional systems and frustrated quantum antiferromagnets and will become an instrumental tool in the discovery of new exotic phases of quantum matter.

DIPC HIGHLIGHT 2020

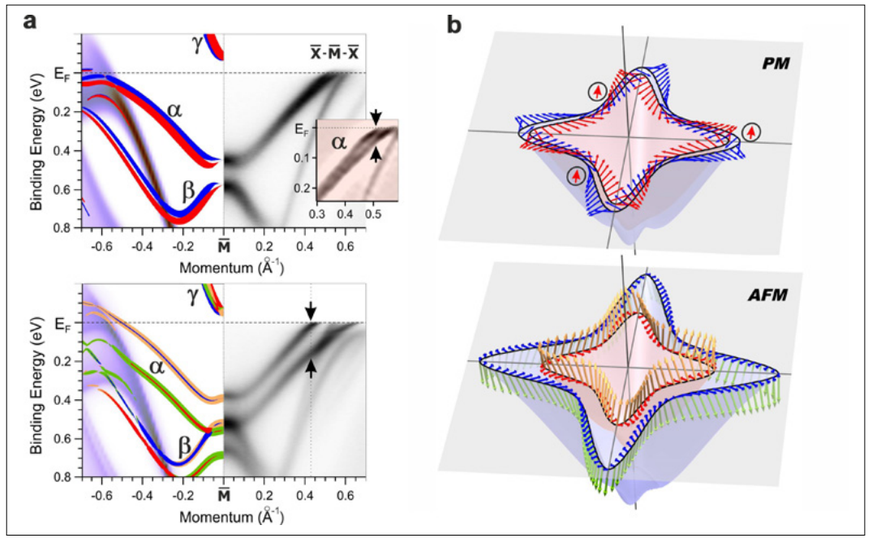
Cubic Rashba effect in the surface spin structure of rare-earth ternary materials

Usachov DY, Nechaev IA, Poelchen G, Guttler M, Krasovskii EE, Schulz S, Generalov A, Kliemt K, Kraiker A, Krellner C, Kummer K, Danzenbacher S, Laubschat C, Weber AP, Sanchez-Barriga J, Chulkov EV, Santander-Syro AF, Imai T, Miyamoto K, Okuda T, and Vyalikh DV
Physical Review Letters 124, 237202 (2020)

At the heart of strongly correlated electron systems are the rare-earth (RE) based compounds, which constantly attract considerable attention due to their exotic bulk properties. The key players in these materials are electrons at the 4f shell, which due to their strong spatial localization cannot participate directly in chemical bonding and maintain their magnetic moments in crystalline solids. The complex interplay between magnetic moments and itinerant electrons including Kondo and RKKY interactions leads to a wealth of extraordinary phenomena as complex magnetic phases, heavy-fermion properties, quantum criticality, valence fluctuations, and many others.

The sophisticated magnetic properties of 4f materials are not only an exciting field for fundamental studies, but they are also of great importance for development of new generation electronic and spintronics devices. For the latter, spin injection and control of magnetic polarization of conduction electrons are of decisive importance, which severely depend on surface properties. Therefore, the surfaces of 4f materials become essential for studies of how the bulk f- driven properties will change when approaching the surface, where in particular, phenomena related to the Rashba spin-orbit coupling emerge. The family of RET_2Si_2 materials, where T is a transitional-metal atom, gives the unique opportunity to investigate such phenomena. Depending on composition, RET_2Si_2 compounds reveal the most prominent aforementioned 4f-derived properties.

This work investigates the electronic and spin structure of rhodium-silicide surface of antiferromagnetic material $TbRh_2Si_2$ by means of momentum- and spin-resolved photoelectron spectroscopy as well as ab-initio calculations and modelling. The most essential result is that the spin structure of the surface-electron state exhibits rather unusual spin texture, which is characterized by a triple winding of the electron spin along the fourfold-symmetric constant energy contour. The studied surface state spreads over four atomic layers that create the non-centrosymmetric surface block Si-Rh-Si-Tb. Within this rhodium-silicide surface, surface electron state experiences both spin-orbit coupling (SOC) due to the Rh atoms and exchange magnetic interaction with the ordered Tb 4f magnetic moments. It was shown that the spin-orbit coupling on the Rh atoms leads to an in-plane spin-momentum locking with the triple winding of the electron spins caused by cubic Rashba mechanism. Its essential property is a fast rotation of the electron spin along the Fermi surface, which is three times faster than in the classical Rashba effect. Moreover, another curious property of this surface state has been unveiled. Namely, its exotic spin structure apparently survives and remains intact when the material transfers from the paramagnetic to the antiferromagnetic phase. In the latter, the Tb 4f magnetic moments become magnetically ordered perpendicular to the surface and create a strong exchange magnetic field. The triple winding of the electron spins within the surface turns out to be rather robust, although the spin-orbit coupling at the Rh atoms is substantially weaker than the out-of-plane exchange field due to the Tb 4f magnetic moments.



Experimental and theoretical insights into the electronic and spin structure of the surface state at rhodium-silicide surface of antiferromagnet $TbRh_2Si_2$. (a) Computed and measured band structure of the surface state for PM (upper panel) and AFM (lower panel) phases. (b) Spin-resolved ab-initio constant-energy contour for the surface states in the PM and AFM phases calculated at the binding energy of 0.23 eV. The points in k-space between which the surface state spin rotates by 2π are shown by the encircled red arrows.

Silicide surfaces of 4f materials offer tunable platforms for fundamental studies of how to integrate semiconductors and magnetic materials, implementing spin functionality in silicon

Finally, this work demonstrates that the silicide Si-T-Si-RE surface of RET_2Si_2 materials can be viewed as a versatile building kit, which allows to design tailored systems for different scenarios by mutually combining fundamental interactions including spin-orbit, Kondo, crystal-electric field, and exchange magnetic interactions and to study the diversity of physics at reduced dimensionality. Another remarkable aspect is that silicide surfaces are intrinsically part of conventional electronics, and therefore, their exploitation in novel materials where two-dimensional carries experience various magnetic interactions in different combinations, becomes important for fundamental studies and may open an avenue for new physics in silicon-based technologies in next-generation electronics.

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Dr. Claire Tonnelé
01/05/2019–30/04/2020
Photon up-conversion via triplet-triplet annihilation in organic aggregates.

Dr. Javier Muñoz Vidal
13/05/2019–15/02/2020
Simulation software and data analysis for xenon detectors.

Dr. Mohamed Ahmed Mohamed Abdelazim Nosir
01/07/2019–Present
Deep eutectic solvents for biomass extraction.

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

Dr. Timo Brändel
15/07/2019–14/06/2020
Investigation on the structural and dynamical properties of macromolecules of diverse nature and architecture in crowded environments.

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

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

Dr. Xavier Monnier
15/11/2019–30/06/2020
Ultra dense/low energy state glasses by agin nanostructured polymers.

Dr. Alejandro Rivero Santamaría
01/01/–31/12/2020
To deepen in the theoretical description of the interactions between small gas molecules and 2D materials using ab initio molecular dynamics methods (AIMD).

Dr. Fernando Aguilar-Galindo Rodríguez
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–Present
Numerical calculations of tunneling conductance in the presents of the Kondo effect.

Dr. Nuno de Sousa Teixeira
30/02/2020–Present
Light scattering in disordered and nonreciprocal media.

Dr. José Angel Martínez González
01/04/2020–Present
Collective dynamics at intermediate length scales in liquids and glass-forming systems by molecular dynamics simulations.

Dr. Khadiza Ali
15/04/2020–Present
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 Fernández Pendás
01/07/2020–Present
Molecular simulations of intrinsically disordered proteins.

Dr. Helena Almazán Molina
01/08/2020–Present
Detector design and analysis for neutrino physics in the "European Spallation Source".

Dr. Mikel Odriozola Gimeno
01/08/2020–Present
Synthesis of fluorophores for detection of SARS-Cov 2.

Dr. Julio Jonás Chaves Montero
01/10/2020–Present
Astrophysics and cosmology.

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

Dr. Sergio Contreras Hantke
04/10/2020–Present
Modelling of galaxy formation physics and its impact on clustering and cosmological parameters.

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

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.

Research Collaborators

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

Dr. Ana Barragán Durán
08/06–07/12/2020
Interaction and bonding of organic sulfur molecules with metal atoms
by low-temperature scanning probe techniques.

Dr. Gabriele Dalla Torre
01/07–31/10/2020
Intrinsically disordered proteins, metal ions and neurodegenerative diseases.

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–Present
Research in Benchmarking of reduced density matrix functional approximations in molecules.

PhD Students

Jordan Ochs
01/10/2016–30/09/2020
Synthesis of cyclic polymers.

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

Peio García Goiricelaya
01/02/2017–29/02/2020
Spinorial structure of the electron-phonon interaction in surfaces with stron relativistic corrections.

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

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

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

Xianpeng Zhang
11/07/2017–14/12/2020
Spin and charge transport in low dimensional systems and hybrid structures.

Mikel Olano Aramburu
01/09/2017–Present
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–Present
Adsorbing atoms and molecules on van der Waals heterostructures.

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

Iñigo Robredo Magro
16/11/2017–Present
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–Present
Electronic and thermal transport through strongly correlated systems
as described by density functional theory.

Quentin Schaeverbeke
15/04/2018–14/01/2020
Dynamical aspects of quantum transport in nanoelectronics.

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

Giovanni Aricò
01/07/2018–Present
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 Zubiría Ulacia
01/11/2018–Present
Triplet states in PDI and related organic molecules.

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

Pablo Herrero Gómez
01/01/2019–Present
Development of hardware an analysis for SABBAT project.

Chiara Devescovi Massussi
07/02/2019–31/08/2020
Topological phases at the frontier of electronic, optical and acoustic materials.

Xabier Tellería Allica
01/06/2019–Present
Statically screened potentials, Hookean systems and quantum dots.

Daniel Muñoz Segovia
01/11/2019–30/10/2020
Charge density wave in transition metal dichalcogenides.

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.

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

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.

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

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

Daniel Muñoz Segovia
01/11/2020–Present
Strongly correlated electron systems and topological materials.

Research Assistants

Lourdes Ondaro Mallea
02/09/2019–26/06/2020

Xabier Díaz de Cerio Palacio
01/10/2019–Present

Leonce Dupays
07/10/2019–31/12/2020

José María Benlloch Rodríguez
01/12/2019–Present

Carmelo Naim
12/12/2019–Present

Mireia Vía Nadal
17/01–30/04/2020

Jon Lafuente Bartaolomé
01/03–30/09/2020

Jon Arrizabalaga Iriarte
01/10–31/12/2020

Aitor Calvo Fernández
01/10/2020–Present

Markel García Ibarluzea
01/10/2020–Present

Daniele Spinoso
05/10/2020–Present

Mikel García Díez
03/11/2020–Present

Haojie Guo
05/11/2020–Present

Adrián Juan Delgado
01/12/2020–Present

Engineers

Dr. Jordi Torrent Collell
16/06/2018–Present

Dr. Eva Oblak
14/09/2020–Present

Rubén González Moreno
21/09/2020–Present

Technical Assistants

Alberto Martínez Pérez
01/11/2018–15/01/2020

Beatríz Romeo Zaragozano
01/11/2018–Present

Daniel Cubero Mimbiela
05/11/2018–05/11/2020

José Luis López Gómez
15/09/2020–Present

Internships

Alex Ciprián López
UPV/EHU, Spain
01/06–31/08/2020
Inclusion of the DIPC in the RedIris SIR2 Single-Sign-On Web.

Mireia Galán Prieto
UPV/EHU, Spain
01/06–31/08/2020
Migration of DIPC web pages to virtual machines.

Markel González de Chavarri Ylla
UPV/EHU, Spain
01/06–31/08/2020
Electronic structure: a real-space model of strong correlation.

Leire Larizgoitia Arcoha
UPV/EHU, Spain
01/06–31/07/2020
Particle physics: searches of coherent neutrino scattering at the european spallation source.

Aitor Díaz Andrés
UPV/EHU, Spain
08/06–7/08/2020
Chemistry: molecular photophysics and optoelectronics.

Maialen Ortego Larrazabal
Leiden University, Netherlands
11/06–10/08/2020
Nanoelectronics: modeling of correlated disorder in 2D topological insulators devices.

Xabier Arrieta Aristi
UPV/EHU, Spain
15/06–31/08/2020
Nanophotonics: Controlling light at the nanoscale with plasmonic antennas.

Errol Drummond
Groningen University, Netherlands
01/07–31/08/2020
Quantum technology: many-body quantum networks and adiabatic quantum computing.

Mikel García Díez
UPV/EHU, Spain
01/07–31/08/2020
Electronic structure: topological properties of metamaterials.

Alvaro Larrarte Arriazu
UPV/EHU, Spain
01/07–31/08/2020
Purchase and commissioning of DIPC information screens.

Mikel Martín Barandiarán
Universidad de Cantabria, Spain
01/07–30/09/2020
Cosmology: computational cosmology and the large-scale structure of the universe.

Julio Pastor Tronch
Universidad de Valencia, Spain
01/07–31/08/2020
Biomedical computer vision: development of open-source computer vision tools for biomedical microscopy data.

Iván Puyol Sayago
Universidad Autónoma de Barcelona, Spain
01/07–31/08/2020
Quantum technology: thermodynamics of non-equilibrium systems.

Edurne Sáenz Parraga
Universidad de Alcalá, Spain
01/07–30/09/2020
Nanophotonics: machine learning applied to the study of light-matter interactions.

Saul Sánchez González
Universidad de Oviedo, Spain
01/07–31/08/2020
Nanoelectronics: quantum transport in nanoscale devices.

Macià Mut Sbert
Universitat de Barcelona, Spain
06/07–04/09/2020
Electronic structure: exciton dynamics in molecular materials.

Asier Orte Nieto
UPV/EHU, Spain
01/09–30/11/2020
Automatic generation of ATLAS Supercomputer usage reports.

Martín Irizar Landa
UPV/EHU, Spain
14/09–14/11/2020
Nanoelectronics: atomic-level simulation of nanoelectronics.

Koldo Descalzo Rosas
UPV/EHU, Spain
01/10–31/12/2020
Generation of automatic reports on BERC connections to the Supercomputer Center.

Julian Nafarrate Andrés
UPV/EHU, Spain
01/10–31/12/2020
Expansion of a relational database for DIPC papers and automation of their analysis.

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

Lorea Sánchez Fernández
UPV/EHU, Spain
01/10–30/06/2021
Experimental project: synchrotron radiation: x-ray radiation meets physics.

Joanes Basurto Merino
UPV/EHU, Spain
26/10–14/02/2021
Estimation of neutrino-nucleus coherent signal in a xenon gaseous TPC at the ESS.

Special Assignments

Aran García Lekue
DIPC Calls for Young Researchers

Geza Giedke and Thomas Frederiksen
DIPC Colloquia

Deung-Jang Choi and Nicolás Lorente Palacios
DIPC Courses

Marek Grzelczak
DIPC Seminars

Fabienne Barroso Bujans
DIPC Summer Internships

Aitzol García Etxarri
DIPC Transdisciplinary Skills Courses

Luca Salassa
DIPC Workshops and DIPC Schools

Gender Equality Committee

Giovanni Aricò

Amaia Arregi Buldain

Silvia Bonoli

Ricardo Díez Muiño

Luz Fernández Vicente

Aitzol García Etxarri

Maia García Vergniory

Elisa Jimenez Izal

Olatz Leis Esnaola

David de Sancho Sánchez

Beatriz Suescun Rodríguez

Visiting Researchers

Long visits

PhD student Naoya Sumi
Institute of Engineering Science,
Tsukuba University, Ibaraki, Japan
01/09/2019–01/03/2020
Surface-supported chemical reactions.

PhD student Eslam Dabbish
University of Calabria, Arcavacata di Rende, Italy
02/09/2019–29/02/2020
Development of photoactivatable
anticancer agents.

Dr. Armando Reyes Serrato
CNyN UNAM, Universidad Nacional Autónoma
de México, Mexico
04/11/2019–18/12/2020
Topological materials.

Prof. Raffaele Resta
Instituto Officina dei Materiali, CNR, Trieste, Italy
01/01–29/02/2020
Geometry and topology in electronic structure.

Prof. Ziya Aliyev
Azerbaijan State Oil and Industry University, Baku,
Azerbaijan
03/01–01/03/2020
Material physics of topological insulators.

PhD student Thomas Richardson
Université Cote d`Azur, Nice, France
06/01–05/03/2020
Constraining the nature of dark matter.

Ece Gülfem Stücker
Istanbul University, Institute of Graduate
Studies In Sciences, Istanbul, Turkey
13/01–08/05/2020
Black hole evolution in a cosmological context.

Prof. Yury Koroteev
Institute of Strength Physics and Materials
Science of Siberian Branch of Russian
Academy of Sciences, Tomsk, Russia
13/01–12/03/2020
Surface electronic structure of systems
with strong spin-orbit interaction.

Prof. Leonid Sviatkin
National Research Tomsk Polytechnic
University, Tomsk, Russia
13/01–12/02/2020
Surface electronic structure of systems
with strong spin-orbit interaction.

PhD student Rishav Harsh
Université de Paris, France
30/01–31/05/2020
Solid-state doping of two-dimensional transition metal dichalcogenides.

Prof. Joseph Richard Manson
Clemson University, South Carolina, USA
01/02–15/03/2020
Electron-phonon interactions near surfaces.

PhD student Raidel Martin Barrios
Institut des Sciences Moleculaires,
Bordeaux, France
01/02–30/03/2020
Dynamics at surfaces.

Dr. Roman Kuzian
Institute for Problems of Materials Science
National Academy of Sciences of Ukraine,
Kiev, Ukraine
02/02–27/03/2020
Time-resolved photoemission from solids.

Dr. Khadiza Ali
CFM-MPC, Donostia/San Sebastán, Spain
14/02–14/04/2020
Phototelectron spectroscopy/STM
of hBN grown on curved Rh and Pt.

Dr. Dmitri Efremov
ILeibnitz Institute for Solid State Physics and
Material Science IFW, Dresden, Germany
16/02–14/03/2020
Electronic excitations and superconducting instability in solids.

Erasmus Elisabetta Contis
Università degli studi di Torino, Italy
18/02–18/08/2020
Development of photoactivatable
anticancer agents.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
23/02–30/06/2020
Electron-phonon interaction
at conducting surfaces; surface dynamics.

Prof. Vladlen Zhukov
Institute of Solid State Chemistry of the Russian
Academy of Sciencies, Ekaterinburg, Russia
25/02–28/03/2020
Electronic band structure and phisico-chemical properties of hyperstoichiometric ferrites
and 3d transition metal formates.

Prof. Oleg Dolgov
Lebedev Physical Institute,
Russian Academy of Science, Moscow, Russia
01/03–30/06/2020
Electronic excitations and superconducting instability in solids.

PhD student Silvia Escayola Gordils
Facultat de Ciències UdG, Girona, Spain
01/03–31/03/2020
Theoretical study of chemical structure and reactivity of aromatic and antiaromatic excited molecular systems.

PhD student Ion Mitxelena Echeverria
UPV/EHU, Donostia/San Sebastián, Spain
01/03–30/06/2020
Development and applications of natural orbital functional theory.

Dr. Rafael Grande Aztatzi
Universidad Autónoma de Tlaxcala, Mexico
01/06–31/07/2020
Molecular dynamics of Al protein interactions.

Prof. Antonio Hernando Grande
Universidad Complutense de Madrid,
Instituto de Magnetismo Aplicado, Madrid, Spain
01/06–31/12/2020
Effect of magnetic fields on
gating of neuron channels.

Prof. Francisco José Garcia Vidal
Universidad Autónoma de Madrid, Spain
01/07–31/07/2020
Light-matter coupling.

Prof. Luis Martin Moreno
Instituto de Física de Materiales de Aragón,
Universidad de Zaragoza, Spain
01/07–31/07/2020
Theoretical nanophotonics.

Prof. Andrey Vasenko
National Research University Higher School of Economics, Moscow, Russia
15/07–31/08/2020
Superconductivity in topologically
nontrivial materials.

Prof. Pilar Hernández Gamazo
Instituto de Física Corpuscular, Valencia, Spain
15/07–14/08/2020
Neutrino physics.

Prof. Pablo Artal Soriano
Universidad de Murcia, Spain
17/07–17/08/2020
Biomedical optics and photonics.

PhD Student Katherine Driscoll
Université Grenoble Alpes and Institut Néel,
CNRS, Grenoble, France
01/09–31/10/2020
Quantum engineering.

Prof. Ceferino Lopez Fernandez
Instituto de Ciencia de Materiales,
CSIC, Madrid, Spain
01/09–30/09/2020
Disorder photonics.

Dr. Adolfo G. Gonzalez Grushin
Néel Institute, CNRS, Grenoble, France
07/09–06/10/2020
Topological phases of matter and non-linear electromagnetic response.

PhD Student Anne Aguirre Gonzalez
University of Cambridge, UK
21/09–23/12/2020
Development of sequence based refined CG model for simulation of phase
separating proteins.

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

Dr. Armando Reyes Serrato
CNyN UNAM, Universidad Nacional
Autónoma de México, Mexico
16/11–18/12/2020
Topological materials.

Short visits

Prof. Juan Faustino Aguilera Granja
Instituto de Física, Universidad Autónoma de San Luis Potosí, México
13/12/2019–05/01/2020
Nanosistemas de baja dimensionalidad y sistemas auto ensamblados.

PhD student David Izquierdo
Villalba, CEFCA, Centro de Física del Cosmos de Aragón, Teruel, Spain
07/01–17/01/2020
Black hole growth and spin evolution.

PhD student Daniele Spinoso
CEFCA, Centro de Física del Cosmos de Aragón, Teruel, Spain
07/01–17/01/2020
Modelling the formation of super-massive black holes at high redshift.

Prof. Edgar Roldán
ICTP, The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy
10/01–24/01/2020
Stochastic thermodynamics.

Prof. Bogdan Andrei Bernevig
Princeton University, New Jersey, USA
12/01–17/01/2020
Topological invariants in electronic structures.

Prof. Javier Rodriguez Vazquez de Aldana
Universidad de Salamanca, Spain
13/01–17/01/2020
Femtosecond direct inscription of 3D photonic structures in glass ceramic materials.

Dr. Petra Bacova
Foundation for Research and tecnology Hellas, Heraldon, Greece
14/01–18/01/2020
Theory and simulation of polymer nanocomposites.

PhD student Diego Romero Abujetas
Instituto de Estructura de la Materia, IEM-CSIC, Madrid, Spain
15/01–29/01/2020
Theory of light scattering in nano-structured highly refractive media.

Dr. Paloma Arroyo Huidrobo
Instituto de Telecomunicaçoes, Instituto Superior Técnico, Universidade Lisboa, Portugal
22/01–24/01/2020
Topoogical photonics.

Dr. Alejandro Gonzalez Tudela
IFF, CSIC Madrid, Spain
22/01–24/01/2020
Topological quantum optics

Dr. Marija Kekic
Universidad de Santiago de Compostela, Spain
24/01–29/01/2020
NEXT.

Dr. Jordi Salvadó Serra
Universitat de Barcelona, Spain
24/01–29/01/2020
NEXT.

Prof. Christian Joachim
CEMES-CNRS, Universite de Toulouse, France and MANA-NIMS, Tsukuba, Ibaraki, Japan
29/01–31/01/2020
The Nanocar Race I and II.

PhD student Jozef Janovec
Brno University of Technology, Brno, Czech Republic
04/02–25/02/2020
Heusler alloys.

Prof. Enrique del Barco
University of Central Florida, Orlando, USA
11/02–12/02/2020
Sub-terahertz spin pumping from an insulating antiferromagnet.

Dr. Claudiu Genes
Max-Planck-Institut für die Physik des Lichts, Erlangen, Germany
12/02–14/02/2020
Cavity-dressed materials.

Prof. Guinievere Kauffmann
Max Planck Institute for Astrophysics, Munich, Germany
15/02–28/02/2020
Galaxy formation.

Prof. Simon White
Max Planck Institute for Astrophysics, Munich, Germany
15/02–28/02/2020
Cosmological simulatons

Dr. Ignasi Pérez Ràfols
LPNHE, París, France
16/02–21/02/2020
Quasar selection methods.

Prof. Amer El-Korashy
The British University Egypt,El Sherouk, Egypt
17/02–20/02/2020
BN Moire structures on Rh(111).

Prof. Antonio García Martín
Instituto de Micro y Nanotecnología - CSIC, Madrid, Spain
17/02–21/02/2020
Chiral and Magneto Optical properties in resonant structures.

Dr. György Hantal
Institute of Physics and Materials Science, University of Natural Resources Vienna, Austria
19/02–22/02/2020
Project planning for Ikerbasque application.

PhD student Olga Matveeva
Moscow Institute of Physics and Technology National Research University, Dolgoprudny, Moscow, Russia
19/02–14/03/2020
Biaxial phonon polaritonic crystals.

Dr. Benjamín Verlhac
Institute Physical And Chemistry Materials De Strasbourg (IPCMS-CNRS), Strasbourg, France
19/02–21/02/2020
Molecules on surfaces.

PhD student Kirill Voronin
Moscow Institute of Physics and Technology, National Research University, Dolgoprudny, Moscow, Russia
21/02–08/03/2020
Trapering graphene plasmons.

Prof. Cornelius Krellner
Goethe University Frankfurt, Germany
23/02–25/02/2020
Magnetically-ordered topological insulators and other intermetallic systems.

Prof. Salvador Miret Artés
CSIC, Instituto de Física Fundamental, Madrid, Spain
23/02–28/02/2020
Electron phonon coupling.

Dr. Charles Downing
Universidad de Zaragoza, Spain
27/02–28/02/2020
Nanophotonics. Plasmonics. Quantum optics.

Prof. Istvan Nagy
Technical University of Budapest, Hungary
02/03–14/03/2020
Higher-order effect in phase shift calculation. Matrix elements between scattering states.

Prof. Björn Trauzettel
Würzburg University, Germany
02/03–04/03/2020
Topological superconductivity.

Dr. Chervin Laporte
Kavli Institute for the Physics and Mathematics of the Universe (IPMU), Chiba, Japan
04/03–07/03/2020
Milky way simulations.

Dr. Federico Mazzola
School of Physics and Astronomy, University of St. Andrews, Scotland, UK
09/03–10/03/2020
Photoemission spectroscopies and their application in solid state and material physics.

PhD student Adrian Martinez Castrillón
Universidad de Santiago de Compostela, Spain
20/04–30/04/2020
Exploring molecular precursors for graphene nanostructures.

Dr. Pierre Anthony Pantaleón Peralta
Instituto IMDEA Nanociencia, Madrid, Spain
10/07–20/07/2020
Correlated effects in graphene superlattices.

Prof. Angel Fernandez Recuero
Jot Down, Sevilla, Spain
15/07–17/07/2020
Colaboration with Jot Down.

Prof. Pavel Jelínek
Institute of Physics of Czech Academy of Sciences, Praga, Czech Republic
25/07–15/08/2020
1D molecular chains on surfaces.

Prof. Paul Soler
University of Glasgow, UK
02/08–05/08/2020
Hyper-Kamiokande, NEXT.

Jacek Generowicz
CERN, Meyrin, Switzerland
06/08–07/08/2020
NEXT.

PhD student Leire Larizgoitia Arcocha
UPV/EHU, Leioa, Spain
08/08–16/08/2020
CNNS at ESS with a Xe TPC.

Dr. Remi Petuya
NEXTMOL, Barcelona, Spain
17/09–18/09/2020
Surface Science.

Personnel

Administration

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

María Tarazona Lorente
Administrative
End of contract 31/12/2020

Outreach

Nora González Lacunza
Outreach Manager

Amaia Arregi Buldain
Outreach Officer

Computing Center

Txomin Romero Asturiano
Computing Center Director

Belén Isla Rodriguez
Computing Center Assistant Director & 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 **Heat engines and Carnot efficiency at the nanoscale**
10/01/2020
Edgar Roldan
ICTP, Trieste, Italy

2 **Quantum optics and simulation with topological photons**
24/01/2020
Alejandro Gonzalez-Tudela
Instituto de Fisica Fundamental (IFF), CSIC Madrid, Spain

3 **Neutrino theory from astrophysics and cosmology**
28/01/2020
Jordi Salvadó
Institut de Ciencies del Cosmos, Universitat de Barcelona, Spain

4 **Cavity-dressed materials**
14/02/2020
Claudiu Genes
Max Planck Institute for the Science of Light, Germany

5 **Atomic-scale spin-sensing with a single molecule at the apex of a scanning tunneling microscope**
20/02/2020
Benjamin Verlhac
Institute Physical And Chemistry Materials De Strasbourg (IPCMS-CNRS), Strasbourg, France

6 **Unconventional effects in Fermi Liquids**
25/02/2020
Dmitrii Efremov
Institute for Solid State Physics, IFW Dresden, Germany

7 Topological nanophotonics
28/02/2020
Charles Downing
Universidad de Zaragoza, Spain

8 The impact of massive satellite accretions on the Milky Way
06/03/2020
Chervin Laporte
Kavli IPMU, Japan

9 The polar surfaces of the delafossite oxides: from massive Rashba spin-splittings to itinerant surface ferromagnetism
09/03/2020
Federico Mazzola
School of Physics and Astronomy, University of St. Andrews, Scotland, UK

10 Structures and formation pathways of nanothreads - a new 1D carbon-based nanomaterial (on line)
27/05/2020
Bo Chen
DIPC, Donostia/San Sebastián, Spain

11 Advanced Nanophotonic Biosensor Platforms for COVID-19 fast diagnostics at the Point-of-need: CoNVat Project (on line)
17/07/2020
Laura M. Lechuga
ICN2, Barcelona, Spain

12 Computational Modelling of Metal-Organic Frameworks (on line)
17/09/2020
Remi Petuya
University of Liverpool, UK

13 ICSP webinar I: Computational Microscopy of SARS-CoV-2 (on line)
13/11/2020
Rommie Amar
University of California, San Diego, USA

14 ICSP webinar II: NMR investigations of the interactions of the N-glycans of the Receptor Binding Domain of the SARS CoV2 spike protein with human lectins (on line)
13/11/2020
Jesùs Jimènez-Barbero
CIC bioGUNE, Bilbao, Spain

15 Biological processes at cellular membranes - new knowledge through the use of neutron and X-ray Scattering (on line)
18/11/2020
Marité Cárdenas
Malmö University, Sweden

16 Porous materials at nanoscale – a neutron scattering insight (on line)
24/11/2020
Margarita Russina
Helmholtz Zentrum Berlin für Energie und Materialien, Berlin, Germany

17 Nuclear Quantum Effects Enter the Mainstream (on line)
30/11/2020
Matthew Krzystyniak
STFC Rutherford Appleton Laboratory, UK

18 Tailoring the interfacial assembly and the mechanical response of colloidal and biological systems (on line)
02/12/2020
Armando Maestro
Institut Max von Laue - Paul Langevin ILL, France

19 Neutron scattering and complementary investigations of fullerene solutions and polymer nanocomposites thin films (on line)
04/12/2020
Timur Tropin
Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia

Colloquia

1 The Nanocar Race I and II
30/01/2020
Christian Joachim
CEMES-CNRS, Université de Toulouse, France
MANA-NIMS, 1-1 Namiki, Tsukuba, Japan

Workshops

20th International Workshop on Computational Physics and Materials Science:
Total Energy and Force Methods 140

NanoNeuro 2020 142

Nanophotonics of 2D Materials (N2D2020) 143

Quantum Thermodynamics of Non-equilibrium Systems 144

International Conference on Electron-phonon Coupling and Thermoelectric Efficiency 145

20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

January 8-10, 2020
Carlos Santamaría Centre, Donostia/San Sebastián
http://totalenergy2020.dipc.org

Organizing Committee
Aran Garcia-Lekue (DIPC, Ikerbasque)
Ivo Souza (CFM-UPV/EHU, Ikerbasque, DIPC)
Ion Errea (CFM-UPV/EHU, DIPC)

This event was the latest in the "mini" series associated with the "Total Energy and Force Methods" workshops, held at ICTP in Trieste every two years. Since 1987 the Trieste workshops have taken place in odd-numbered years, alternating with the mini workshops, held each even-numbered year in a different location. The most recent workshops of the "mini" series took place in Madrid (2000), Tenerife (2002), Paris (2004), Cambridge (2006), Bonn (2008), Shanghai (2010), Barcelona (2012), Lausanne (2014), Luxembourg (2016), and Cambridge (2018).

The workshop focused on the most recent developments in the field of electronic structure methods from the first-principles perspective, their diverse applications and mathematical foundations. The numerous approaches that are developed and used in the electronic-structure community provide the foundation for computing many physical and chemical properties of solids, liquids, and low-dimensional systems. However, there are numerous challenging applications for which the level of approximation is insufficient or where computational costs are prohibitive for accurate quantitative prediction of material properties. Therefore, continued efforts are devoted to the improvement of existing methods, and the development of new methods.

Invited Speakers
Antia Botana (Arizona State University, USA)
Matthew Foulkes (Imperial College London, UK)
Xavier Gonze (Université Catholique de Louvain, Belgium)
Myrta Grüning (Queen's University Belfast, UK)
Efthimios Kaxiras (Harvard University, USA)
Eduard Matito (DIPC, Spain)
Miguel Marques (Martin-Luther-University Halle-Wittemberg, Germany)
Lorenzo Monacelli (Sapienza University of Rome, Italy)
Titus Neupert (University of Zurich, Switzerland)
Thomas Olsen (Technical University of Denmark)
Nick Papior (Technical University of Denmark)
Silvia Picozzi (Università degli Studi di Chieti, Italy)
Cheol-Hwan Park (Seoul National University, South Korea)
Andrew M. Rappe (University of Pennsylvania, USA)
Alexandre R. Rocha (State University of São Paulo, Brazil)
Ivana Savic (Tyndall National Institute, Ireland)
Thibault Sohier (Ecole Polytechnique Fédérale de Lausanne, Switzerland)
Massimiliano Stengel (Institut de Ciència de Materials de Barcelona, Spain)
Ilya Tokatly (UPV/EHU, Spain)
Roser Valentí (Goethe University Frankfurt, Germany)
Xiangang Wan (Nanjing University, China)
Binghai Yan (Weizzmann Institute of Science, Israel)
Jakub Zelezny (Czech Academy of Sciences, Czech Republic)

NanoNeuro 2020

June 24-25, 2020
Online
http://nanoneuro2020.dipc.org

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

The conference aimed to help nucleate the emerging field of research at the intersection of Nanoscience and Neuroscience and provide a forum for experts from both areas to interact.

Due to COVID-19, this symposium, organized by the NeuroTechnology Center at Columbia University along with the Donostia International Physics Center (DIPC), and supported by the Kabli Foundation, was held online.

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 was organized in thematic sessions with keynote and invited talks.

Invited Speakers
Javier Aizpurua (CFM-CSIC, Donostia/San Sebastián)
Laura Ballerini (SISSA Institute, Trieste, Italy)
Louis Brus (Columbia University, NY, USA)
Jose Carmena (UC Berkeley, CA, USA)
Fernando Cossio (UPV/EHU, Donostia/San Sebastián)
Jennifer A. Dionne (Stanford University, CA, USA)
Naomi Halas (Rice University, TX, USA)
Luis Liz Marzan (BiomaGUNE, Donostia/San Sebastián)
Wei Min (Columbia University, NY, USA)
Hongkun Park (Harvard University, MA, USA)
Jacob Robinson (Rice University, TX, USA)
Mike Roukes (Caltech, CA, USA)
Ken Shepard (Columbia University, CA, USA)
Rafa Yuste (Columbia University, CA, USA)

Nanophotonics of 2D Materials (N2D2020)

July 13-16, 2020
Online
http://n2d-2020.dipc.org

Organizing Committee
Alexey Nikitin (DIPC, Ikerbasque)
Tony Low (U. Minnesota)
Luis Martín-Moreno (ICMA, CSIC - U. Zaragoza)

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 at providing a setting where researchers from diverse fields can convene; classical and quantum optics; excitons, phonons and plasmons; far-field and near field spectroscopies such as, 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
Pablo Alonso Gonzalez (University of Oviedo, Spain)
Andrea Alu (CUNY Advanced Science Research Center, USA)
Harry Atwater (California Institute of Technology, USA)
Dmitri Basov (Columbia University, USA)
Federico Capasso (Harvard University, USA)
Monica Felicia Craciun (University of Exeter, UK)
Sergey Ganichev (Regensburg University, Germany)
Irina Grigorieva (University of Manchester, UK)
Francisco Guinea (IMDEA, Spain)
Rainer Hillenbrand (Nanogune, Spain)
James Hone (Columbia University, USA)
Frank Koppens (ICFO, Spain)
Alexey Kuzmenko (University of Geneve, Switzerland)
Xiao Lin (Nanyang Technological University, Singapore)
Michal Lipson (Columbia University, USA)
Lukas Novotny (ETH Zurich, Switzerland)
Sang-Hyun Oh (University of Minnesota, USA)
Marco Polini (Italian Institute of Technology, Italy)
Miriam Vitiello (National Research Council, Italy)
Valentyn Volkov (Moscow Institute of Physics and Technology, Russia)
Hugen Yan (Fudan University, China)

Quantum Thermodynamics of Non-equilibrium Systems

October 13-16, 2020
Online
http://qtdneq20.dipc.org

Organizing Committee
Tineke van den Berg (DIPC)
Aurelia Chenu (DIPC, Ikerbasque)
Geza Giedke (DIPC, Ikerbasque)
Dario Bercioux (DIPC, Ikerbasque)

The workshop focused on new developments in the understanding of quantum thermodynamics in non-equilibrium systems, with emphasis on the meso- and nanoscopic scale. Special attention went to possible implementations of proof-of-principle experiments of systems working in the quantum regime.

Invited Speakers
Sahar Alipour (Aalto University, Espoo, Finland)
Janet Anders (University of Exeter, UK)
Alexia Auffèves (University of Grenoble Alpes, France)
Adolfo del Campo (DIPC, Ikerbasque, Spain)
Irene D'Amico (University of York, UK)
Geraldine Haack (Université de Genève, France)
Ronnie Kosloff (The Hebrew University of Jerusalem, Israel)
Jorge Kurchan (LPS, L'École normale supérieure-PLS, Paris, France)
Rosa López (Universitat de les Illes Balears, Mallorca, Spain)
Eric Lutz (ITP, University of Stuttgart, Germany)
Jukka Pekola (Aalto University, Espoo, Finland)
Peter Samuelsson (Lund University, Sweden)
Jörg Schmiedmayer (TU Wien, Austria)
Janine Splettstößer (Chalmers University of Technology, Göteborg, Sweden)

International Conference on Electron-Phonon Coupling and Thermoelectric Efficiency

November 11-13, 2020
Online
https://www.uik.eus/en/live-online-congress-international-conference-electron-phonon-coupling-and-thermoelectric-efficiency

Organizing Committee
Roberto D'Agosta (UPV/EHU, Ikerbasque)
Davide Donadio (University of California - Davis)
Thomas Frederiksen (DIPC, Ikerbasque)

This workshop aimed at:

- Bringing together the communities working on thermoelectricity and electron-phonon coupling, to establish fruitful connection between them.
- Fostering collaborations between the experimental and theory groups on these outstanding problems.
- Bringing, once again, San Sebastian and the Basque Country at the forefront of an important scientific and technological problem, thus fostering the internationalization of our research activities.
- Providing the young members of the audience, both PhD students and postdocs, a good reference for their investigation and shaping of their research activities on this field by bringing together some of the most prominent scientists.

The conference, articulated in invited and contributed talks, in general, tried to follow the three tracks: methodology development, experimental results and new material discovery.

Invited Speakers
Alejandro Goñi (CSIC-ICMAB, Spain)
Antonios M. Alvertis (Univ. of Cambridge, UK)
Bin Xu (Soochow University, China)
Charles Sievers (Univ. of California - Davis, USA)
Darshil Chodvadiya (Univ. of Baroda, India)
Dmitry Turchinovich (Univ. Bielefeld, Germany)
Fabian Pauly (OIST, Japan ; Univ. of Ausburg, Germany)
Feliciano Giustino (Univ. of Texas - Austin, USA)
Francesco Mauri (Univ. of Rome "La Sapienza", Italy)
Gemma Solomon (Univ. of Copenhagen, Denmark)
Ismael Ali (Lancaster University, UK)
Ivana Savic (Tyndall Cork, Ireland)
Jagoda Slawinska (Univ. of Groningen, Netherlands)
Jelena Sjakste (Ecole Polytechnique, France)
Madhubanti Mukherjee (IISc Bangalore, India)
Mads Brandbyge (DTU Lyngby, Denmark)
Marco Bernardi (Caltech, USA)
Marco Buongiorno Nardelli (Univ. of North Texas, USA)
Marisol Martin Gonzales (CSIC-Madrid, Spain)
Matthieu Verstraete (Univ. of Liege, Belgium)
Michele Simoncelli (EPFL, Switzerland)
Nahual Sobrino (UPV/EHU, Spain)
Nicolas Agrait (Univ. Autónoma de Madrid, Spain)
Orla Surgeoner (Queen's Univ. Belfast, UK)
Paz Vaqueiro (Univ. of Reading, UK)
Prafulla Jha (Univ. of Baroda, India)
Roxana Margine (Binghamton University, USA)
Thibault Sohier (Univ. of Liege, Belgium)
Venkat Kapil (EPFL, Switzerland)
Zhen Li (Univ. of Warwick, UK)
Zhimei Sun (Beihang University, China)

Higher Education

DIPC School

AEBIN Photochemistry School 2020 148

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DIPC School

AEBIN Photochemistry School 2020

September 7-9, 2020
Online
https://www.uik.eus/es/live-online-aebin-photochemistry-school-2020

Organizing Committee
Luca Salassa (DIPC, Ikerbasque)
Alessio Terenzi (University of Palermo, DIPC)
Álvaro Martínez (DIPC)
Juan Gurruchaga (DIPC, CIC biomaGUNE)
Laura Mazzei (DIPC, CIC biomaGUNE)

Scientific Committee
José Ruiz (Universidad de Murcia)
Patrick Gámez (Universidad de Barcelona, ICREA)
Josefa González (Universidad de Granada)
Ana I. Matesanz (Universidad Autónoma de Madrid)
Luca Salassa (DIPC, Ikerbasque)

The AEBIN Photochemistry School 2020 provided an introductory overview of the use of photochemistry and photobiology in health-related sciences and other disciplines. In their lectures, international experts in these research areas discussed basic principles and advanced applications of light in chemistry, biology and medicine. The School was principally directed to early career researches such as PhD students and postdocs, who had the opportunity to present their work as poster and oral communications. These were evaluated by the lecturers and the best of each were awarded with prizes.

Invited Speakers
Claudia Turro (University of Ohio, USA)
Gilles Gasser (Chimie ParisTech, France)
Santi Nonell (Universitat Ramon Llull, Barcelona, Spain)
Paolo Melchiorre (ICIQ, Tarragona, Spain)
Peter Sadler (University of Warwick, England, UK)
Olalla Vázquez (Philipps Universitat Marburg, Germany)
José Ruiz (University of Murcia, Spain)
Luca Prodi (Università di Bologna, Italy)
Virginia Martínez Martínez (UPV/EHU, Spain)
Ruben Esteban (CFM-CSIC, DIPC, Spain)
David Casanova (DIPC, Ikerbasque, Spain)

DIPC Course

Moiré patterns and metamaterials from two dimensional systems

February 18-24, 2020
DIPC, Donostia / San Sebastián
http://dipc.ehu.eus/dipc-courses/introduction-to-2-dimensional-system

Organizer
Prof. Francisco Guinea López (DIPC, IMDEA Nanociencia)

Stacks of atomically thin systems allow for the formation of periodic structures with lattice lengths significantly larger than lattice constant of the constituent materials, which are typically a few angstroms.

These patterns are due either to the mismatch in the lattice constants of the materials in the stack, or to the relative rotation of neighboring layers in the stack. The lack of defects in many two dimensional materials, especially in graphene, makes possible the observation of novel phenomena related to these new structures.

The series of two 90 minute lectures reviewed the current status of theory and experiments on Moiré superlattices built from two dimensional materials. Emphasis was made on the electronic structure of these systems, and the new phases it leads to.

Transferable skills course

Career development:
Take the step from academia to industry

June-July, 2020
DIPC, Donostia/San Sebastián

Sofi Facal and Manuela Bercioux
Skills for Science and Industry

For many young researchers the knowledge and skills gained during the academia education are the foundation of a successful career in the private sector.

Nevertheless there are several hurdles that can stop young researchers form stepping into industry positions. These challenges range from a simple lack of knowledge of possible job options to practical challenges like how to prepare an appealing industrial resume or how to communicate in a job interview.

This training aimed to aid the participants in overcoming these hurdles. To achieve this, the main focus of the training was:

- Broaden the spectrum: Career options for PhDs in industry.
- Transferable Skills: What are they? How to get them, how to show them?
- Apply to industry: The resume, letter, and further application documents.
- The job interview: How to prepare for it and how to succeed.
- Individual feedback and interview coaching for each participant.

Theses

Spin-dependent and non-adiabatic phenomena related to the electron-phonon interaction in nanostructures with strong relativistic corrections.
Peio García Goiricelaya
03/04/2020
Supervisors: Asier Eiguren Goyenechea and Idoia García de Gurtubay Galligo

Electron correlation in density matrices and Coulomb holes.
Mireia Vía Nadal
17/07/2020
Supervisor: Eduard Matito Gras

Photon emission and quantum transport in nanoplasmonic cavities.
Quentin Schaeverbeke
04/09/2020
Supervisors: Thomas Frederiksen, Fabio Pistolesi and Rémi Avriller

Synthesis and characterization of cyclic polyethers with controlled orientation of the dipolar moment along the chain contour.
Jordan Ochs
19/09/2020
Supervisor: Fabienne Barroso Bujans

Computational methods to solve many-body problems from first principles: a focus on the electron-phonon interaction.
Jon Lafuente Bartolomé
05/11/2020
Supervisors: Asier Eiguren Goyenechea and Idoia García de Gurtubay Gálligo

Spin- and valley-dependent transport in hybrid systems and 2D Dirac materials.
Xianpeng Zhang
02/12/2020
Supervisors: Sebastián Bergeret and Miguel Angel Cazalilla Gutierrez

The NEXT experiment: DAQ, backgrounds and medical applications.
José María Benlloch Rodríguez
18/12/2020
Supervisors: Juan José Gómez Cadenas, Paola Ferrario and Javier Muñoz Vidal

Master's Degree Program

UPV/EHU Research Master's in Nanoscience

DIPC, along with CIC nanoGUNE, collaborates in the official postgraduate 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 155 students having obtained their Master's degree. Almost 50% 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: ehu.eus/en/web/master/master-nanoscience

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