
dipc2022
Donostia International Physics Center

ON THE COVER

THE NEW HYPERION SUPERCOMPUTER STORAGE

The next DIPC supercomputer, Hyperion, will be available to Basque researchers in 2023, becoming the most powerful supercomputer ever active in the Basque Country. Its amount of memory, cores and GPUs makes it the best possible facility to face very demanding computational problems. On the cover is an image of the Hyperion's storage, where the results of computational jobs can be written at high speed using distributed file systems.

Image Hyperion supercomputer | Paula Arbide

2022

DIPC ACTIVITY REPORT

More is Different Different is More

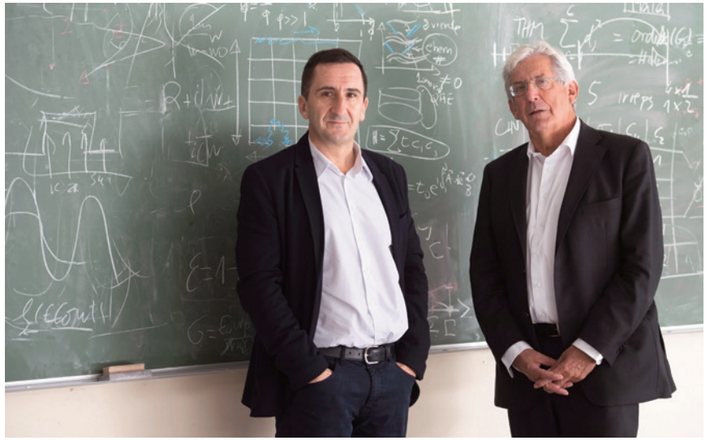
In 1972, the Nobel-winning theoretical physicist Phil Anderson published an article in the Science magazine entitled "More is different". In his text, now a classic, Anderson defends an anti-reductionist vision of science, in which greater levels of complexity bring about the birth of new, emergent, properties that cannot be deduced from those of the preceding simpler levels. The bottom line of Anderson's argument is that a progressive quantitative increase implies, at some point, a qualitative difference. Simply put, Anderson claims that *more is different*.

In the past five years, DIPC's scope has widened and we have experienced substantial growth in many areas. In terms of scientific production, a clear indicator is the increase in the number of articles; from 327 in 2018 to 450 in 2022. During the same period, the number of employees at DIPC has more than duplicated, the budget has increased by a factor of 56%, and the number of active grants from the European Research Council grants has grown from 5 to 7.

In accordance with Anderson's arguments, the recent growth of DIPC has also engendered a qualitative change. DIPC is assuming a new role as a driving force in many scientific, technological, and institutional initiatives. For instance, we host the DIPC Supercomputing Center that is being transformed into a general supercomputing service, open to all Basque research centers by mandate of the Department of Education of the Basque Government. DIPC coordinates the IKUR Strategy of the Basque Government in High Performance Computing and Artificial Intelligence, as well as the IKUR Strategy on Quantum Technologies (IKUR-Quantum). IKUR-Quantum has been used as a framework to establish an ambitious collaboration agreement between Basque institutions and IBM. This collaboration ensures the installation of an IBM System One quantum computer in Donostia / San Sebastián. DIPC will be playing a leading role in the IBM collaboration. DIPC is also the Basque coordinator of the Spanish Complementary Plan on Quantum Communications, as well as the Basque coordinator of the Spanish Complementary Plan on Advanced Materials. Last but not least, DIPC leads several large-scale international collaborations in neutrino physics (NEXT and nuESS) and is making relevant contributions to HyperKamiokande and some other initiatives.

However, the transformation of quantity into quality in the recent life of DIPC does not tell the full story. In parallel with the growth in size of the center, DIPC's research lines have evolved and diversified. Since its establishment in 2000, DIPC developed activity in several fields of physics, materials sciences, and chemistry, including condensed matter physics, atomic and molecular physics, chemical physics, computational physics, computational chemistry, photonics, theoretical chemistry, photophysics, and photochemistry. All of these subjects are now grouped into two big areas of research that we call QUANTUM and NANO. During the last few years, DIPC has also opened new research lines in computational cosmology, astrophysics, and neutrino physics, which are now gathered under the generic term of COSMOS. Incipient lines of research on the physics and chemistry of biological systems as well as on the connections between nanoscience and neuroscience are arising as well. They are included in the research area LIFE. All these research areas at DIPC are not isolated systems, but rather open ones with overlapping borders. They contribute to create a dynamic and interconnected research environment.

We have discussed that the scope of the research now performed at DIPC has broadened, enriching the expertise found at the Center, and improving the impact of the generated knowledge. The diversity of research topics under the same roof is proving to be immensely fruitful in stimulating outstanding interdisciplinary projects among DIPC scientists from diverse backgrounds. Moreover, it has helped establish valuable institutional relationships between DIPC and other research centers both locally and internationally. At DIPC, we are aware that more is different but we also assert that different is more.



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

The diversity of research topics under the same roof is proving to be imensely fruitful in stimulating outstanding interdisciplinary projects among DIPC scientists from diverse backgrounds.

Within DIPC's Board of Partners, both public institutions and private organizations coexist. The joint support from entities of different character reinforces the position of DIPC. We embrace difference and diversity in the workforce and we empower our scientists with freedom and trust. We are fully committed to the responsibility of sharing science with society. We believe that developing creative science communications programs in collaboration with academic and cultural agents from different fields and backgrounds is crucial to promoting human culture as a whole. In every one of these aspects, different is more.

Let's finish here by saying that the success of DIPC in 2022 was only made possible thanks to the dedication, hard work, and enthusiasm of our entire scientific, technical, and administrative community. They are the true driving force behind the center's achievements and progress. ■

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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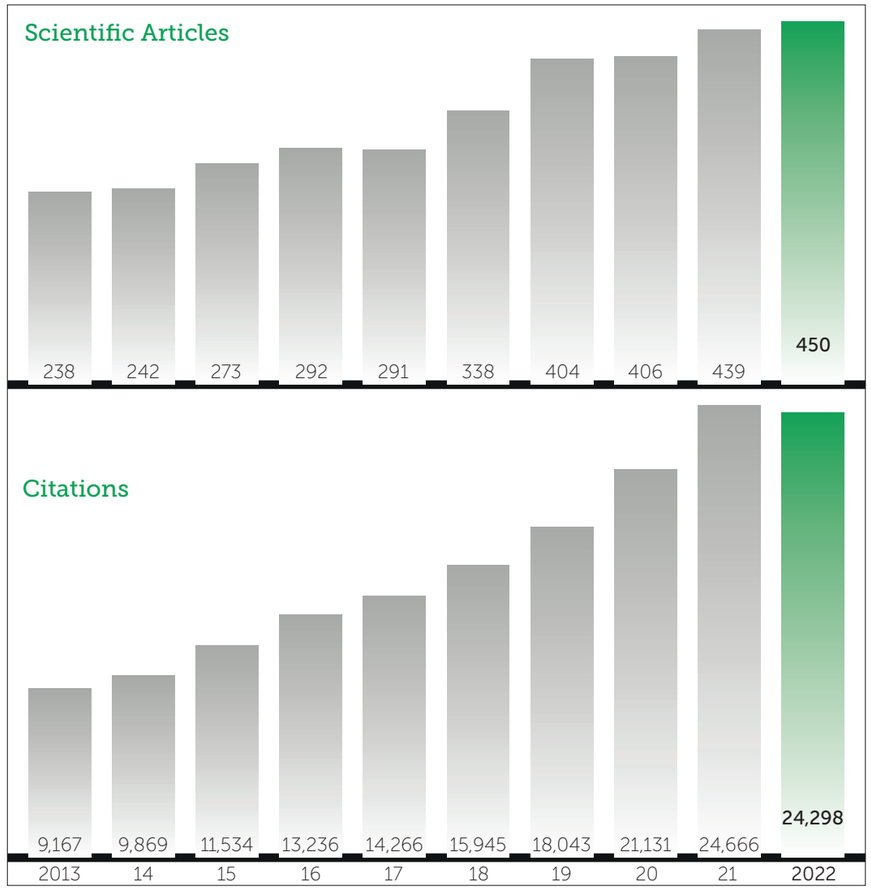
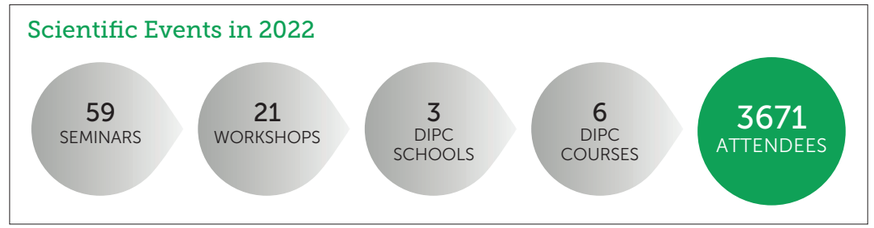
Research Activity at a Glance

Research activity is back to its normal course, and following the trend of previous years, DIPC's scientific production and international impact continues on an upward trend. In 2022, **450 scientific articles** were published, similar to the numbers in 2021, but with a larger impact in regard to other science indicators. Since DIPC first started activity 24 years ago, we have published a total of **5,297 ISI articles** and have received more than **206,000 citations**.



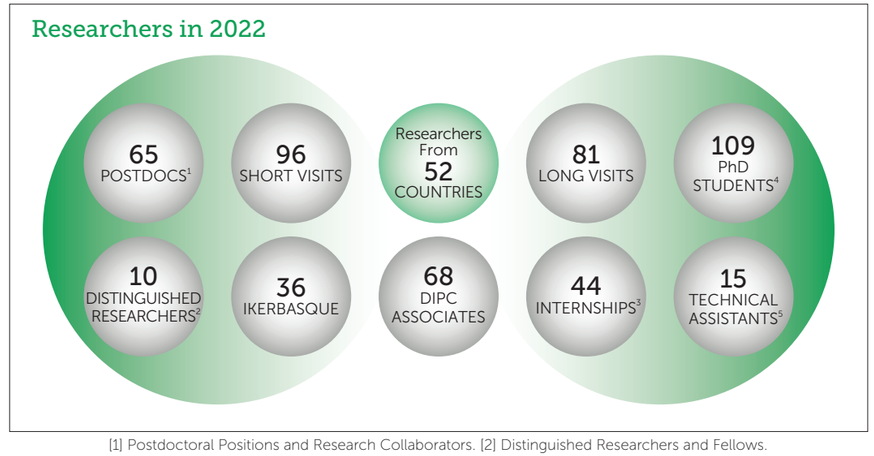
Source Web of Science Core Collection (all years and all indexes, 07/04/2023)



In addition to doing research, DIPC's annual strategic agenda of actions foster exchange with scientists from around the world. Our Scientific Events include several formats. Seminars, given by international experts, cover research topics of particular interest to our community. Our Workshops highlight specific subjects of interest. And both the DIPC Schools and the Courses, especially aimed at young researchers, focus on learning particular skills. In 2022 most of the programmed activities were held in person, but in order to reach a larger audience many of them were also streamed live.

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

The core of the DIPC Community is made up of senior scientists and technicians, as well as PhD students and postdoctoral researchers. These young scientists complete their training and hone their expertise at the Center. In addition, DIPC counts on DIPC Associates, who are hired by other institutions but develop part of their research activity at DIPC. Last but not least, our scientists act as hosts for a large number of international visiting researchers that greatly contribute to DIPC's scientific activity. All in all, the vibrant energy of our research community creates a stimulating environment that fosters creativity.



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

DIPC Supercomputing Center

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

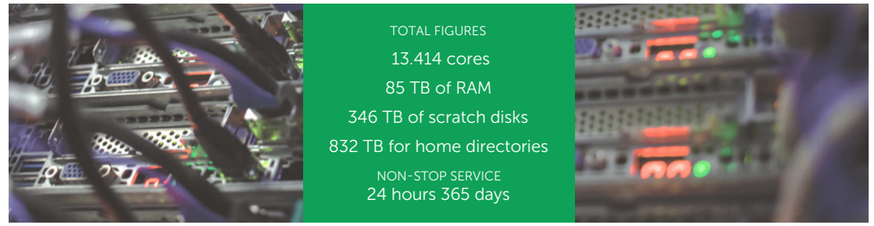
Computational physics and chemistry are among the strongest research fields in the Basque Country and the Supercomputing Center is one of its key resources. In recent years the Supercomputing Center has also started offering its services to other type of research lines related to Cosmology, Genetics,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

DIPC Supercomputing Center's team.

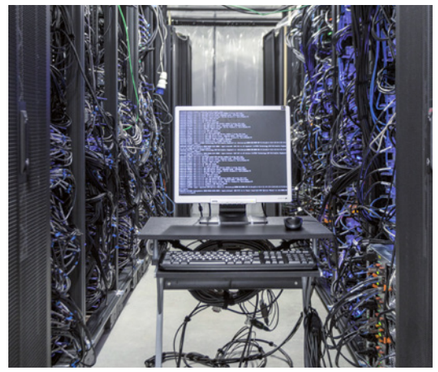
Current computing resources

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

As of 2022, 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). The ATLAS resources include NVIDIA Tesla P40 and GeForce RTX 3090 technology for GPGPU programming. With more than 13,000 cores and 80 TB of RAM, is one of the more powerful supercomputers in Spain. In addition, the Center has begun to build this year a new supercomputer named HYPERION, that will be three times more powerful than ATLAS.



More than 400 researchers from DIPC and other research centers of the Basque Country such as the UPV/EHU, the CSIC-UPV/EHU Materials Physics Center, Ikerbasque, CIC nanoGUNE, CIC Biomagune, IIS BioDonostia, Tecnalia, Tecnun, or ESS Bilbao and several BERCs like BCAM, BCBL, BCMaterials, Biofisika, Achucarro, or BC3 used this computational infrastructure in 2022.



Science Communication

DIPC places great emphasis on Science Communication, and has developed a strong science outreach program over the years. As we returned to normalcy, citizens returned to public activities with enthusiasm, and in 2022 participation rates have exceeded all expectations. In total, we have organized **134 events**, both in person and online, with the direct participation of over **27,211 people**. Additionally, these events received over **100,000 views** from various media outlets. It is gratifying to witness people continuing to respond passionately to our educational and cultural programs.

The return to the velodrome, one of the most exciting moments of 2022.

Top@DIPC Encounters–Zientziarekin Solasean!

On March 25, we celebrated at Eureka! Zientzia Museoa the XII edition of Top@DIPC–Zientziarekin Solasean!, an encounter between top-level scientists and high school students from the Basque Country. In this edition, the students had the opportunity to talk to the physicist **Albert Fert** (Nobel Prize in Physics 2007), the chemist **María Vallet-Regí** (King Jaime I Award for Basic Research in 2018) and the anthropologist **María Martinón** (director of CENIEH), in an encounter moderated by the physicist **Pedro Miguel Echenique**. The invited scientists talked about their professional careers and answered the questions posed by the students.

The main goal of this encounter is to promote vocations for scientific and technological careers among Basque youth, as well as to kindle passion for knowledge in them.

The event was supported by the Basque Government's Department of Education and was organized by DIPC in collaboration with Eureka! Zientzia Museoa, as well as the special collaboration of Telefónica, that awarded a prize to the most interesting question raised among all the participants.

25/03/2022| Eureka! Zientzia Museoa
Top@DIPC Encounters Dialogue with top scientists
Albert Fert Université Paris-Saclay, UPV/EHU, DIPC
María Martinón CENIEH
María Vallet-Regí UCM
Moderated by **Pedro Miguel Echenieque**
President of DIPC

Hosts:
Larraitz Etxeberria Eureka! Zientzia Museoa
Javier Benito Director Telefónica Euskadi
Amaia Esquisabel Director of Research, Department of Education of the Basque Government

CINEMA AND SCIENCE

With the aim of transmitting cinematographic and scientific culture, the fifth edition of the 'Cinema and Science' cycle organized jointly by DIPC, the Basque Film Archive, and the San Sebastian International Film Festival took place from January to March 2022. The 10 films screened in different venues were preceded, as is tradition, by inspiring presentations and subsequent discussions led by renowned scientists. The sessions took place, as usual, at Tabakalera (Donostia), the Bilbao Fine Arts Museum and the Le Sélect cinema in Saint Jean de Luz. In addition, for the first time, Artium Museum in Vitoria, that hosts since October the Basque Film Archive's regular program and the Golem-Baiona cinemas in Pamplona joined the cycle; this last, thanks to an agreement with this private cinema and the collaboration of the Pamplona Planetarium. Overall, **over 3100 people** participated in the multiple screenings.

General Sessions

Films projected in
(1) Vitoria-Gasteiz (2) Donostia/San Sebastián
(3) Bilbao (4) Pamplona (5) Saint Jean de Luz

The Prize (Mark Robson, 1963)
(1) 13/01/2022 (2) 14/01/2022
(3) 15/01/2022 (4) 18/01/2022
Physicist **Pedro Miguel Etxenike**, UPV/EHU, DIPC

Moby Dick (John Huston, 1956)
(1) 27/01/2022 (2) 28/01/2022
(3) 29/01/2022 (4) 01/02/2022
Biologist **Juan Ignacio Pérez Iglesias**, UPV/EHU, DIPC

Hope (Maria Sødahl, 2019)
(1) 03/02/2022 (2) 04/02/2022
(3) 05/02/2022 (4) 08/02/2022
Molecular biologist **María A. Blasco**, CNIO
Biologist **Ana Zubiaga**, UPV/EHU
Biochemist **Sara Manzano Figueroa**, Biodonostia

Gorillas in the Mist (Michael Apted, 1988)
(1) 10/02/2022 (2) 11/02/2022
(3) 12/02/2022 (4) 15/02/2022
Biologist **Joana Vitorica Onaindia**, World Rural Forum
Biologist **Arantza Acha**, UNESCO Etxea
Organized in collaboration with *Emakumeak Zientzian*

Demon Seed (Donald Cammell, 1977)
(1) 17/02/2022 (2) 18/02/2022
(3) 19/02/2022 (4) 22/02/2022
Computer scientist **Olatz Arbelaitz Gallego**, UPV/EHU
Computer scientist **Elena Lazkano**, UPV/EHU

The Man in the White Suit (Alexander Mackendrick, 1951)
(1) 24/02/2022 (2) 25/02/2022
(3) 26/02/2022 (4) 01/03/2022
Chemist **Xabi López**, UPV/EHU, DIPC
Chemist **Jon Mattin Matxain**, UPV/EHU, DIPC

Ikarie XB 1 (Jindrich Polák, 1963)
(1) 03/03/2022 (2) 04/03/2022
(3) 05/03/2022 (4) 08/03/2022
Chemist **Fernando Cossío**, UPV/EHU, Ikerbasque
Computer scientist **Txomin Romero**, DIPC

Inception (Christopher Nolan, 2010)
(1) 10/03/2022 (2) 11/03/2022 (3) 12/03/2022
(4) 14/03/2022 (5) 15/03/2022
Physicist **Aitzol García-Etxarri**, Ikerbasque, DIPC
Physicist **Ricardo Díez Muiño**, DIPC, CFM (CSIC-UPV/EHU)
Physicist **Amaia Arregi**, DIPC

Contact (Robert Zemeckis, 1997)
(1) 17/03/2022 (2) 18/03/2022
(3) 19/03/2022 (4) 22/03/2022
Astrophysicist **Silvia Bonoli**, Ikerbasque, DIPC
Astrophysicist **Marcos Pellejero**, DIPC

La guerre du feu (Jean-Jacques Annaud, 1981)
(1) 24/03/2022 (2) 25/03/2022 (3) 26/03/2022
(4) 28/03/2022 (5) 29/03/2022
Paleoanthropologist **María Martinón**, CENIEH
Archeologist **María José Iriarte**, Ikerbasque, UPV/EHU
Physicist **Ricardo Díez Muiño**, DIPC, CFM (CSIC-UPV/EHU)
Historian **Joxean Fernández**, Basque Film Archive

Special Sessions

In collaboration with *Emakumeak Zientzian* initiative, the event around the 11th of February celebrated the International Day of Girls and Women in Science with the screening of *Gorillas in the Mist* (Michael Apted, 1988). Additionally, a special session of the documentary *Picture a Scientist* was programmed as satellite event at the Science and Technology Park of Gipuzkoa to celebrate the 8th of March, the International Day of Women. The film portraits three female scientists and their intimate journey through years of subtle slights and brutal harassment.

Picture a Scientist (Ian Cheney, Sharon Sattuck, 2020)
08/03/2022

School Sessions

Special morning sessions for students were organized in San Sebastian, Bilbao and Vitoria-Gasteiz. The film selected on this occasion was *Apollo 11* (Todd Douglas Miller, 2019), a documentary film about the 1969 Apollo 11 mission, the first spaceflight from which humankind walked on the Moon. The screening was presented by scientists and science disseminators.

Physicist **Naiara Barrado-Izagirre**, UPV/EHU
Physicist **Santiago Pérez-Hoyos**, UPV/EHU
Physicist **Javier Aizpurua**, CFM CSIC-UPV/EHU, DIPC
Scientific journalist **Valentina Rodríguez**, DIPC
Physicist **Aran Garcia-Lekue**, DIPC

Bilbao
02/02/2022 *(In Basque)* 03/02/2022 *(In Spanish)*

Donostia/San Sebastián
02/03/2022 *(In Basque)* 03/03/2022 *(In Spanish)*

Vitoria-Gasteiz
09/03/2022 *(In Basque)*

Photo of the presentation of the program at the press conference: Ricardo Díez Muiño (DIPC), Xabier Garat (Le Sélect), Joxean Fernández (Filmoteca Vasca), Bingen Zupiria (Basque Government Minister of Culture and Language Policy), Pedro Miguel Etxenike (DIPC), Edurne Ormazabal (Tabakalera), José Luis Rebordinos (Festival de Cine de San Sebastián), Silvia García Lusa (Museo de Bellas Artes) and Beatriz Herráez (Artium).

WOMEN IN SCIENCE

11-18/02/2022

Emakumeak Zientzian project has been growing year on year. DIPC was one of the promoting institutions involved from the very beginning in the project and has participated ever since in the organization. In 2022, **17 entities**, constituting a significant representative sample of the Basque Country's science and technology base, jointly organized the 6th edition. The participation reached overall **over 5100 people**.

"PIZTU! Emakumeon energia" represented by Eidabe theater group.

The most noteworthy news about the project in 2022 was the recognition with the first **STEAM Euskadi Prize 2022** and the **Special Mention Award for Gender Perspective** by the Basque Government's Department of Education. The project was selected among 137 applications submitted to the call for proposals.

The objective of this initiative is making the activity of women in science visible, breaking with the typically male roles attributed to scientific-technical activities, and encouraging the choice of scientific careers among girls and teenagers. With these objectives in mind, the organizer entities run a joint program of activities to mark the **International Day of Women and Girls in Science**, which is celebrated every year on February 11. **38 activities** aimed at all audiences, including workshops, public talks, family experiments and virtual visits were put together thanks to this highly cooperative alliance. Emakumeak Zientzian 2022 had the substantial support of the **Provincial Council of Gipuzkoa** and **Fomento San Sebastián**, along with other collaborating entities.

Activities in which DIPC was directly involved as organizer are collected afterwards:

11/02/2022 | Carlos Santamaría Library
Encounter Emakumeak Zientzian Public lectures
General public

10/02/2022 | Artium Vitoria-Gasteiz
11/02/2022 | Donostia/San Sebastián
12/02/2022 | Bilbao
15/02/2022 | Baiona-Golem Pamplona
Cinema and Science
"Gorillas in the Mist" screening
Joana Vitorica Onaindia World Rural Forum
Arantza Acha UNESCO Etxea
General public

13/02/2022 | Science and Technology Park of Gipuzkoa
"PIZTU! Emakumeon energia"
Eidabe theater group Theater play
Families with children
with the special support of EDP Foundation

14-18/02/2022 | CIC biomaGUNE, CIC nanoGUNE, DIPC/CFM, Faculty of informatics UPV/EHU and BCBL
Do you know a female scientist?
Workshops and guided tours
Schools

15/02/2022 | DIPC/CFM, Polymat and CIC biomaGUNE
The power of experience
Hands-on experiments
Women ages +55

17/02/2022 | Victoria Eugenia Club Aretoa and Streamed Live
Women Scientists of Yesterday and Today Public Lectures
General public

Invited scientists and honored scientists:
Clara Martin, BCBL, **Suzanne Noël**
Miryam Criado Gonzalez, Polymat, **Margarita Salas**
Miren Aristizabal, Ceit, **Emily Warren Roebling**
Ana Álvarez Yenes, CIC nanoGUNE, **Stephanie Kwolek**
Carmen Martín Valderrama, CIC nanoGUNE, **Donna Strickland**
Olga Ibáñez Solé, Biodonostia, **Alexandra Elbakyan**

08/03/2022 | Science and Technology Park of Gipuzkoa
Cinema and Science special session
"Picture a Scientist"
Scientific Community

For more information visit
https://emakumeakzientzian.eus

PRIDE IN SCIENCE

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

To celebrate Pride in Science Day 2022, we hosted the "Looking inside to get outside" event on November 21 at the Victoria Eugenia Club auditorium. The event was dedicated to our own community and an informal work-coffee session with the aim of getting to know and building an LGTBIQA+ community in the STEM environment of Donostia/San Sebastián was organized. We invited all those members working in the STEM field in Donostia/San Sebastián to participate in this event, offering them a safe space to exchange ideas, opinions, and experiences.

Later, we built a summary of what was discussed in the event, capturing all the contributions and bringing together the experiences, opinions and aspirations of everyone who participated in the event. One of the main conclusions is that we all want to build a community in our immediate environment.

SURF AND SCIENCE

The program *Donostia, Zientzia Hiria* was launched in 2022 by Donostia Kultura, in collaboration with DIPC and the Chair of Scientific Culture of UPV/EHU, to examine under the magnifying lens of science some iconic places and topics related to San Sebastian.

The first edition was dedicated to *Surf and Science* (*Surfa eta Zientzia*), due to its strong roots in the city and its surroundings, and for the various and interesting processes that can be examined under the light of scientific disciplines.

The program of activities included a series of monthly conferences from January to March at **Okendo Kultur Etxea**, in which renowned figures of science and surfing addressed the subject from different perspectives, such as physics, meteorology, health, sports and engineering. These conferences were all in Basque, free of charge and aimed at all audiences.

In addition, five totems with attractive infographics, made by NorArte Studio in collaboration with the Chair of Scientific Culture of UPV/EHU, rotated through different parts of the city explaining the science behind the waves and the technology that moves surfboards.

Finally, an online contest was launched consisting in answering a series of questions accessible through a QR code printed in the Surf and Science totems displayed in the city. The prize was a surf class with an introduction on scientific concepts applied to surfing, offered by Zurriola Surf Eskola in collaboration with DIPC.

26/01/2022 | Okendo Kultur Etxea
History of a wave Public lecture
Physicist **Maia García Vergniory** DIPC
Surfer **Kepa Acero**
General public

23/02/2022 | Okendo Kultur Etxea
Impact of surfing in physiology and Health
Public lectures
Sports physician **Julen Ucin** UPV/EHU
PhD in Sport Sciences **Aitor Santisteban**
Universidad de Deusto
General public

23/03/2022 | Okendo Kultur Etxea
The perfect wave and surfboards shaping
Public lectures
Meteorologist **Onintze Salazar**
Euskalmet/Tecnalia
Pukas project manager **Adur Letamendia**
General public

21/05/2022 |
Zurriola Surf Eskola and Zurriola beach
Surf and science prize class
Lecture and practical lesson
Physicist **Aran García-Lekue** DIPC, Ikerbasque
Zurriola Surf Eskola staff
Contest winners

PUBLIC LECTURE By Maria A. Blasco

The prestigious molecular biologist Maria A. Blasco, scientific director of the National Cancer Research Center (CNIO), arrived in San Sebastian as a special guest of the fifth edition of Cinema and Science. DIPC took the occasion to organize a public lecture to give a broader audience the opportunity to learn about her frontline research, considered pioneer in the field of molecular aging associated with cancer.

04/02/2022 | Tabakalera
The origin of diseases Public lecture
Molecular biologist **Maria A. Blasco** CNIO
General public

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 during the last 12 years. These activities have been done in collaboration with the San Telmo Museum, Donostia Kultura, Tabakalera and the Vice Rectorate of the Guipúzcoa Campus of the University of the Basque Country.

During 2022, the following activity was carried out:

COMPLEX NETWORK METHODS APPLIED TO CULTURAL ANALYTICS

Throughout 2021 and 2022, we have forged a solid and fruitful collaboration with the digital humanities laboratory, The CulturePlex Lab, in London, Canada. We have signed a three-year collaborative project that includes hiring a PhD student and a postdoc to conduct an intense research program. We propose to use the formalism of complex networks, data mining and artificial intelligence to understand the conditions that allow the emergence of geniuses and revolutionary ideas. This research project aims to deepen the analysis and understanding of cultural networks around iconic people and revolutionary ideas to characterize the structure and dynamics that allow their emergence. In 2022, the first results were already published in high-impact specialized magazines.

For more information visit
www.mestizajes.es

ON ZIENTZIA

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

For its 12th edition, a record number of 93 works were received for the contest, representing an unprecedented level of interest. Participants exhibited gender parity, reflecting a positive trend in promoting diversity and inclusivity. Videos were submitted in Basque, Spanish and English. While the majority of the submissions originated from the Basque Country, it is gratifying to note that several contributions came from far-flung regions such as Colombia, Mexico, and Argentina, among others.

The 2022 award ceremony was held on June 17 at Tabakalera.
In each category, the following works were awarded by the jury:

BEST DISSEMINATION VIDEO
Argitazpen artifizial... naturala?
Alain Sorazum, Alfredo Rodríguez, Kimberlyn Fonseca Pérez and Morgane Goyens
Science ilustrators from Lanius Animatics

BEST VIDEO IN BASQUE
Iruzurra
Joseba Zabala and Aitziber Zurutuza

YOUNG PRIZE
El no Nobel de Rosalind Franklin
High school students from the School Luis Amigó from Mutiloa, Navarre

SPECIAL MENTIONS
Partículas celtíberas
Nuria Gordillo García, PhD in Physics and researcher at CMAN
¿De qué están hechas las estrellas?
Astrophysicists Tatiana Cazorla Cabezas and Esteban Melchor Gordo

POPULAR PRIZE
La droga del siglo XXI
2nd year of compulsory secondary education of the School Doña Jimena of Gijon, Asturias

For more information visit
www.onzientzia.tv

SESSIONS FOR KIDS: San Sebastian International Film Festival

16, 19-23/09/2022
Ikastetxeak Belodromoan, Anoeta Velodrome

After two years of virtual sessions due to the pandemic, 13.200 children aged between 6 and 11 finally returned to the Velodrome to enjoy the San Sebastian Film Festival screenings for kids, co-organized by the San Sebastian International Festival, DIPC and the Basque Film Archive since 2019. With the slogan *City of Cinema, City of Science*, the goal of this collaboration is to convey a positive image of science to the local schoolchildren while highlighting the city's strong connection to scientific research.

The return to Velodrome was full blast, with the screening of *Terra Willy: Planeta ezezaguna*, an animated film directed by Eric Tosti about a boy who, after a space accident, must survive on an unexplored planet, with the help of a robot and an alien creature. The screening of the movie, dubbed into Basque, was preceded by the unexpected appearance of the social robot Pepper, who interacted with the public and even made them dance.

The presence of Pepper in the Velodrome was possible thanks to a collaboration with the Robotics and Autonomous Systems (RSAIT) research group of the University of the Basque Country (UPV/EHU), led by the professor and researcher Elena Lazkano, and also composed by computer scientists and researchers Igor Rodriguez and Unai Zabala.

HIGH SCHOOL VISITS

Since 2014, DIPC and the Materials Physics Center (CSIC–UPV/EHU) put together the *DIPC/CFM visit program* with an open call for high schools to visit our research centers with the objective of inspiring scientific careers and showing our daily activities. In 2022, both on-site and virtual visits were arranged in order to respond to the high demand from the schools. Overall, more than 1100 students from 34 high schools participated. The visits agenda included two special visits organized within the *Egokitu orientation program* (UPV/EHU). Moreover, students on microcomputer systems from Zubiri Manteo pay a special visit to DIPC Supercomputing Center, and winners from *Zientzia Azoka* (Elhuyar) visited our research center, having the opportunity to get to know scientists from our community.

DIALOGUE ON NEURORIGHTS Human rights: a reference framework for neurotechnology and digital technologies

28/07/2022
San Telmo Museum

San Telmo Museum (STM) and DIPC co-organized a round table to discuss about *Human rights: a reference framework for neurotechnology and digital technologies*. The session started with a presentation about the so-called "neurorights" by the renowned neuroscientist **Rafael Yuste**, director of the NeuroTechnology Center at the University of Columbia and a board member of the Neurorights Foundation. The introduction then was followed by a multidisciplinary dialogue involving different young profiles, that included: **Leire Mendiluce**, physician from the University of Deusto, and **Mikel Edeso**, non-profit sector journalist, both members of the Aranzadi Science Society; and also the biomedical engineer **Teresa Celaya**, PhD student at DIPC and member of the NanoNeuro project research team. The session was moderated by **Aitzol García-Etxarri**, leader of the DIPC nanophotonics group and co-founder of the Basque Nanoneuro Network (B3N).

The session was part of the "Challenges" series, in which **San Telmo Museum** addresses contemporary issues of interest for our society, creating platforms for reflection and debate. **266 people** attended the event in person and online through the STM youtube channel, with more than **800 online views** accumulated to date.

NEW WAYS OF SCIENCE

This cycle is co-organized by the Ernest Lluch Cultural Center of **Donostia Kultura** and DIPC, with the aim of bridging the gap between our scientific endeavors and society at large. Members from DIPC research community present the hot-topics and milestones in the field of Physics and related disciplines, as well as significant historical accomplishments, in a lucid and captivating manner.

In 2022, we organized the following lectures:

17/05/2022
Quantum computing today
Román Orús, DIPC, Ikerbasque, Multiverse Computing

25/10/2022
NANONEURO the power of nanoscience to explore the frontiers of neuroscience
Aitzol Garcia-Etxarri, DIPC, Ikerbasque

SCIENCE WEEK

10-12/11/2022
Tabakalera

As every year DIPC, CIC nanoGUNE and the Materials Physics Center (CFM CSIC-UPV/EHU) participated in the Science Week of the University of the Basque Country (UPV/EHU), with the incorporation of Polymat as part of the team. In this edition we retrieved the usual stand with hands-on experiments on materials science and nanoscience. The program also included a specific hands-on workshop for children focused on the experimentation of the tiny world and its visualization.

10-12/11/2022
Stand "Exploring the world of materials"

12/11/2021
Eskalatu zure mundua (Scale your world)
Workshop for children (+6)

Additionally, some of our scientists participated in the monologue event **Zientzia Club** that took place at Okendo Cultural Center.

12/11/2022
Zientzia Club

Bestiario estelar
Daniel López DIPC

Metales en medicina
Luca Salassa DIPC, Ikerbasque

Desemborronando el Universo. No veo bien ese millón de galaxias, ¿me las puedes acercar?
Marcos Pellejero Ibañez DIPC

CLOUDS OF POLLEN: Art and Science at Tabakalera

Tabakalera and DIPC co-produced the science and art project *Clouds of Pollen. Data, living material*, an artistic installation that studies the storage of digital data in living beings, created by the collective *Grow Your Own Cloud* in collaboration with the artificial life scientist and DIPC's visiting researcher Steen Rasmussen.

The artists Monika Seyfried and Cyrus Clark from the collective *Grow Your Own Cloud*, have investigated the possibilities of DNA data storage in plants since 2017. In this work, they conducted an exchange with Steen Rasmussen, with the goal of understanding the potential for living systems to interact with artificial life. This dialogue materialized in the form of an art installation displayed on the second floor of Tabakalera from October 6 to November 10, 2022.

Clouds of Pollen. Data, living material is part of the *Art and Science* collaboration agreement signed between DIPC and Tabakalera, by which artists and scientists address key issues in current scientific research to explore future conceptions of life, identity, humanism, as well as sustainability, among others.

06/10-10/11/2022 | Tabakalera
Clouds of Pollen. Data, living material
Art Installation
Grow Your Own Cloud collective
Monika Seyfried and **Cyrus Clark**
Physicist **Steen Rasmussen** University of Southern Denmark
General public

JOT DOWN SCIENCE 2022

11-12/06/2022
Conference and Exhibition Center, Jaca

Jointly with the popular cultural magazine Jot Down, since 2015 DIPC organizes annually the Jot Down Science outreach contest. In the last years, new collaborators have joined in, such as the University of Seville, the museum Laboratorium of Bergara, and the Canfranc Underground Laboratory. The award ceremony takes place in the *Jot Down Science Event* traditionally celebrated in Seville. In 2021, the event took place for the first time in San Sebastian and in 2022 travelled to Jaca in the Pyrenees.

The program of the event included outreach talks, round tables on invisibility treated from social and scientific perspectives, the above mentioned contest awards ceremony and a guided tour to the Canfranc Underground Laboratory, a singular scientific infrastructure where DIPC's NEXT experiment is based.

11/06/2022
Lectures by **Mucuy Guevara** (Universidad Nacional Autónoma de México), **Javier S. Burgos** (Universitat Jaume I), **Javier Aizpurua** (CFM CSIC- UPV/EHU, DIPC) and **Sergio Parra**.

Round table on *Invisibility in Science*
Participants: **Aitzol García-Etxarri** (DIPC), **Olatz Leis** (DIPC) and **Ana Nuñez** (DIPC)
Moderator: **Mª Carmen Escámez** (Universidad de Sevilla)

Round table on *Artificial Intelligence: the invisible brain*
Participants: **Juan Prieto**, **Jose Valenzuela** (Universidad de Barcelona), **Yolanda Morató** (Universidad de Sevilla) and **Irene Larraz** (periodista en Newtral)

Round table on *The invisible universe*
Participants: **Patricia Parra** (LSC), **Nuria Rius** (IFIC/Universidad de Valencia), **Quim Palacio** (LSC) and **Francesc Monrabal** (DIPC, Ikerbasque)

Interview by **Juan José Gómez Cadenas** (DIPC, Ikerbasque) and **Ángel Fernández** (Jot Down) to **Lorena Escudero** (University of Cambridge)

Jot Down 2022 Science Outreach Contest

Best Scientific Dissemination Essay
El poder invisible del lenguaje | **Lorena Pérez**

Best Science Fiction Narrative Award
El ojo que no ves | **Carlo Frabetti**

Award for the Best Scientific Illustration
The Invisible | **Maddi Astigarraga Bergara**

Best Photography Award
Sustainable Energy | **Aldo Luján Zanetti**

DONOSTIA WeekINN 2022

DIPC regularly collaborates in the Innovation Week 'Donostia WeekINN' that Fomento of San Sebastian organizes every end of October. In 2022, this collaboration included the following activities for both the general public and schools organized in collaboration with other institutions:

25/10/2022 | St Patrick's English School
Hands-on workshop on Materials Science and Nanoscience

26/10/2022 | Donostia Aquarium
Women scientists of yesterday and today
Featuring *Emakumeak Zientzian* 2022 edition's speakers and honored scientists

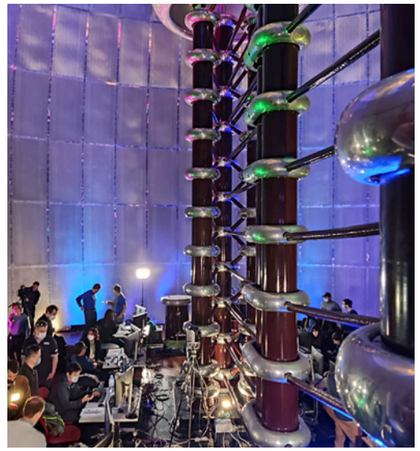
In addition, one school visit within de annual program carried out jointly with CFM was scheduled in the framework of WeekINN, where several students could visit our centers and get to know our diverse community.

NANOCAR RACE II

24-25/03/2022
Toulouse

The tandem from Donostia/San Sebastián and Santiago de Compostela **SANCAR** (CFM, DIPC and CIQUS-USC) was one of the 8 teams certified to participate in the second edition of the International Nanocar Race II that took place at Toulouse for 24 h non-stop in the framework of the European project MEMO (MEchanics with MOlecules).

In the Nanocar Race, the vehicles are molecules driven by the tip of a tunneling microscope over a gold surface as a circuit. All teams competed simultaneously from the same room in Toulouse, controlling their nanocar remotely. The aim of the competition is to advance knowledge in the development and manipulation of molecular machines.



The design and construction of **SANCAR molecule** was carried out by **Diego Peña** and his team from CiQUS. SANCAR was made up of 128 carbon, hydrogen and oxygen atoms. It had a pentaphene chassis, eight phenyl wheels and two ester groups as propellants. The theoretical design of the system was done by **Nicolás Lorente** and **Roberto Robles**, from CFM and DIPC, whereas the experimental setup and training was carried out at the nanophysics laboratory of CFM and DIPC, with a team composed by **Jan Patrick Calupitan, Martina Corso, Paula Ángulo, Tao Wang, Alejandro Berdonces,** and **Dimas G. de Oteiza**, a DIPC associated who is currently developing his research at CINN in Asturias. Finally, **Lucia Vitali** from CFM, provided the STM microscope where the Sancar race track was located while the pilots controlled remotely the molecule from Toulouse.

STEAM Sare

As part of the STEAM Euskadi Strategy promoted by the Department of Education of the Basque Government via Innobasque, STEAM sare is a network that connects schools with research centers, universities and companies with the goal of providing a realistic, positive and diverse picture of the research professions, as well as to fostering STEM related vocations. DIPC is currently part of the network, and in particular during 2022 we participated in a pilot project to include the "A" of art within the STEAM curricula.

During the project, the activity "*Gravitating Bodies*" was co-created by a team comprised of Egoitz Etxeandia and Nerea Casas, teachers from the Lauaxeta Ikastola (Amorebieta-Etxano, Bizkaia), scientists Marcos Pellejero and Sergio Contreras, both from DIPC´s Astrophysics and Cosmology group, as well as artist Saioa Olmo. They all participated together in the conception and development of the activity and the resulting didactic unit. The pilot test was carried out with students from Lauxeta Ikastola and was very satisfactory. As a result, a new didactic unit aimed at students in the 2nd year of High School is now available to investigate the concept of gravity through a group dynamic that mixes science, art and creativity.

In addition, a group of DIPC researchers, as well as the director of DIPC Supercomputing Center participated in the second edition of the STEAM Sare Orientation Fair that took place on October 18 in Orona Building (Hernani).

OTHER COLLABORATIONS

In addition to our outreach program, every year we sponsor and support different initiatives with the participation of our researchers. In 2022, these initiatives include *Scientific Lifes* organized by Eureka! Zientzia Museoa to inspire scientific vocations among the new generations of students, *Aranzadi's Astronomical Days*, public outreach lectures organized by Aranzadi Foundation, and *Pint of Science*, an international initiative which is also celebrated in San Sebastian offering science dissemination informal talks by local scientists in bars across the city.

WOMEN AND SCIENCE

The goal of 'Women and Science' program launched by the Gipuzkoa Provincial Council and DIPC in 2021 is to promote the presence of women in science of excellence, combining the scientific quality of DIPC and the objective of the Council to pushforward gender equality in all areas and especially in those where this inequality is most evident.

In the framework of this initiative, DIPC organized inspiring career sessions for young female researchers at DIPC, and visits by our female scientists to schools, with the aim of encouraging STEM vocations, especially among girls.

24-25/03/2022 DIPC Seminar room
Inspiring Careers: a round table with Isabel Márquez
Institute of Astrophysics of Andalusia (IAA-CSIC)

23/03/2022 Toki Ona BHI
Fostering scientific vocations with chemist Claire Tonnele DIPC

27/05/2022 DIPC Seminar room
Inspiring Careers: a dialogue with Laila Saad Beni-Suef University, Egypt
Laila Saad was hosted by DIPC within the program *Science by Women* of the Women for Africa Foundation thanks to the support of the Gipuzkoa Cooperates program of the Gipuzkoa Provincial Council

27/10/2022 Lasalle Zumarraga BHI
Fostering scientific vocations with astrophysicist Silvia Bonoli DIPC, Ikerbasque

DIPC 2022 THE YEAR IN MEDIA

107	44	8	+600
newspaper articles	radio impacts	television appearances	online Impacts

Equality at DIPC

Emakumeak Zientzian

In 2022, Emakumeak Zientzian, an initiative promoted by DIPC together with local partners, received several awards including the **STEAM Euskadi Award** granted by the Department of Education of the Basque Government and Innobasque. During 2022, more than **100 researchers from 17 scientific institutions** made possible nearly **40 activities** aimed to permeate an egalitarian scientific culture throughout society to include children, families, teenagers, adult women, and teachers.

Emakumeak Zientzian organizers and scientists at the event in Tabakalera in Donostia/San Sebastián.

The STEAM Euskadi Award is given in recognition of the journey made by Emakumeak Zientzian since its first edition in 2017, and for the effort of the people and organizations involved in its progress. Emakumeak Zientzian also won Special Mention for Gender Perspective in the category of most innovative STEAM education initiative delivered by the Education Department of the Basque Country and Innobasque. Additionally, this project has also received Special Recognition from Fomento San Sebastian at the awards ceremony of the 9th edition of Innovation Week in 2022.

Emakumeak Zientzian has an extensive program of activities aimed at the general public celebrated close to the date of February 11th which is the International Day of Women and Girls in Science. It focuses on particularly vulnerable groups in order to promote equal access and professional development in STEM disciplines, giving visibility to women researchers in the Basque Country and breaking the typically male roles attributed to scientific-technical activities.

Thanks to this initiative, a network of scientists committed to internal change in scientific and technical organizations has been created to break the gender gap, and address the leaky pipeline by which progressive reduction in women's participation is globally happening in STEM fields at different stages of career development. We wish to achieve full and equal professional development for all people.

Equality Plan

In 2022, we continued our implementation of the First Equality Plan initiated by DIPC in 2020 and designed a framework comprising of four principal areas which were identified as significant challenges during the diagnosis process: organizational culture, workforce diversity, sexual harassment in the workplace, and work-life balance.

Creating an inclusive organizational culture with diverse gender leadership and transparency at its core is one of the principal objectives we have been working on at DIPC. Significant actions are shared with the community every year. In addition, we are aware of the importance of promoting diversity and inclusivity internally with the use of language which is implemented throughout our different communication channels.

To promote a diverse workforce, we have been raising awareness and enhancing the visibility of underrepresented researcher collectives (gender, ethic background, etc.) as role models in local community events. The Pride in Science event which we celebrate every November 18th together with CFM and CIC nanoGUNE aims at giving visibility to the LGBTQIA+ community in science and actively contributes to the demolition of stereotypes. Furthermore, a specialized program entitled Women and Science has been established in partnership with the Gipuzkoa Provincial Council. Its primary objective is to promote the careers of high profile female scientists. Finally, in collaboration with the Gipuzkoa Provincial Council's Gipuzkoa Coopera program, DIPC hosts an African researcher for several months through the Science by Women initiative, led by the Women for Africa Foundation. To end each year, the Learn Africa scholarship is offered jointly by CFM and DIPC to a female African student for enrolment in the Master in Nanoscience program at UPV/EHU. People who participate in these programs are regularly involved in activities within the community and the education system.

In 2021, a **protocol against harassment** was established to guarantee and maintain a dignified work environment for all DIPC workers, free of violence in general and free of violence against women and minorities, that may occur both in and outside of the physical space of DIPC, as well as those that could take place through virtual or symbolic means of communication. The implementation of the protocol, which has been in place for two years now, has been one of the most important milestones of our Equality Plan. Every year, awareness and prevention campaigns are carried out involving our community.

Egyptian scientist Laila Saad during the presentation of Science by Women at the Gipuzkoa Provincial Council.

Protocol Against Harassment

DIPC's 1st Equality Plan

One of our next challenges is to work in the area of **work-life balance** with specific actions to develop a work environment that facilitates the integration of work, family and private life for both women and men.

Personnel Segregated by Gender

	Total Staff	Men / Women
Direction & Management		
Directors	4	0% / 100%
Managers	4	75% / 25%
Total	8	37% / 63%
Scientific		
Pre-Docs	74	32% / 68%
Post-Docs	47	19% / 81%
Distinguished Researchers	9	33% / 67%
Ikerbasque Research Fellows	6	17% / 83%
Ikerbasque Research Associates	11	19% / 81%
Ikerbasque Research Professors	16	7% / 93%
Engineers	7	29% / 71%
Technical Assistants	5	20% / 80%
Total	175	25% / 75%
Technical & Administrative		
Administrative Staff	12	67% / 33%
IT Personnel	6	50% / 50%
Outreach Personnel	2	100% / 0%
Total	20	65% / 35%
TOTAL	**195**	29% / 71%

Associates and Visiting Researchers

	Total Staff	Men / Women
Strategic Level		
DIPC Associates	69	23% / 77%
Visiting Researchers	7	29% / 71%

Data as of 31/12/2022. DIPC includes the non-binary gender definition, but none has been recorded to date.

Scientific Highlights

DIPC HIGHLIGHT 2022

Interlayer coupling of a two-dimensional Kondo lattice with a ferromagnetic surface in the antiferromagnet $CeCo_2P_2$

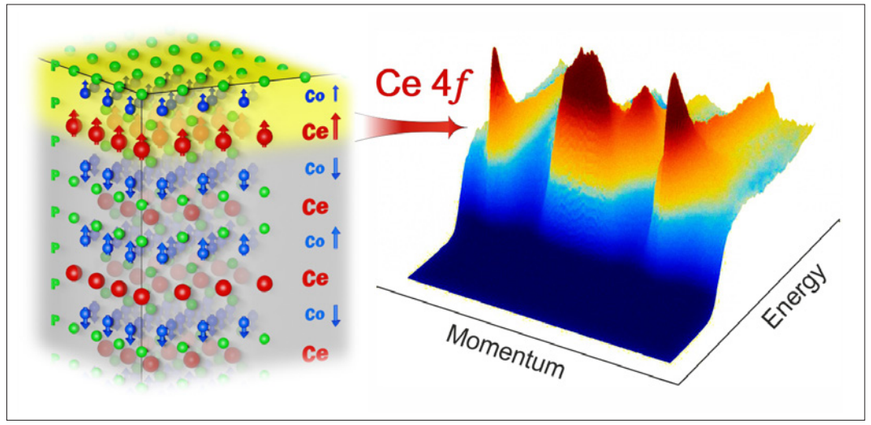
Poelchen G, Rusinov IP, Schulz S, Guttler M, Mende M, Generalov A, Usachov DY, Danzenbacher S, Hellwig J, Peters M, Kliemt K, Kucherenko Y, Antonov VN, Laubschat C, Chulkov EV, Ernst A, Kummer K, Krellner C, and Vyalikh DV
ACS Nano 16, 3573 (2022)

The rare-earth based materials are at the heart of strongly-correlated electron systems, and permanently attract considerable attention due to the exotic bulk properties. The surfaces of such materials, however, often do not receive as much attention as their bulk. However, it is reasonable to anticipate that the f-driven physics at the surface can be even much richer and more compelling than in the bulk. Lack of inversion symmetry and spin-orbit coupling (SOC), appearance of surface-electron states and resonances, relaxation and reconstruction, as well as strong changes of the crystal-electric field near and at the surface are the driving forces for novel f-driven phenomena, phases and temperature scales that are in remarkable difference to those in the bulk.

A strong interest represents the surfaces of quasi-2D rare-earth-based materials, which contain the magnetically active f- and d- sublattices and which experience mutual interactions. In this paper, we report on a comprehensive investigation of the P-Co-P-Ce surface of the quasi-2D material $CeCo_2P_2$, where Co reveals ferromagnetic order within the ab plane, which stack antiferromagnetically along the c axis with a rather high TN of 440 K.

Our measurements indicate the Ce sublattice is rather passive in the bulk and behaves tetravalently. However, at the P-Co-P-Ce surface, the Ce layer becomes magnetically active. This is because of the symmetry breaking, bond reduction and magnetic field resulting from the uncompensated ferromagnetic Co layer within the P-Co-P-Ce surface block, which leads to the partially occupation of the Ce 4f shell. Our momentum-resolved photoemission (ARPES) measurements indicate a strong admixture of the Ce 4f states to the itinerant electrons bands near the Fermi level including the spin-split bands caused by exchange interactions at the Co layer. The temperature-dependent ARPES spectra reveal strong changes of the 4f intensity near the Fermi level in accordance with the Kondo scenario.

The obtained results allow concluding that Ce sublattice within the P-Co-P-Ce surface reveals a Kondo lattice behavior. Our theoretical results indicate that the emerged 2D Kondo lattice couples ferromagnetically to the ordered Co lattice within this surface block.



Visualization of the emergence of two-dimensional Ce Kondo lattice which experiences a strong mutual interlayer coupling with two-dimensional ferromagnetic layer of Co within the P-Co-P-Ce surface of tetravalent antiferromagnet $CeCo_2P_2$. The red arrows indicate the induced magnetic moments on Ce atoms.

Our findings show how rich and diverse the f-driven properties at the surface of the material without f-properties in the bulk can be

Overall, our findings show how rich and diverse the f-driven properties at the surface of the material without f-properties in the bulk can be. Our results make a call for detailed studies of the properties emerging at the surfaces of many strongly correlated Ce, Eu, and Yb materials with layered, quasi-2D structure. They also bear strong implications for how novel functional and quantum materials can be devised using thin layers of f-materials as building blocks. In such systems, different combinations of fundamental interactions like SOC, exchange magnetism, heavy-fermion behavior, unconventional superconductivity and others, originating from distinct atomic layers can be realized. Thus, combining these interactions with one another gives the opportunity to predict and create novel materials with new functionalities.

DIPC HIGHLIGHT 2022

Role of the magnetic anisotropy in atomic-spin sensing of 1D Molecular Chains

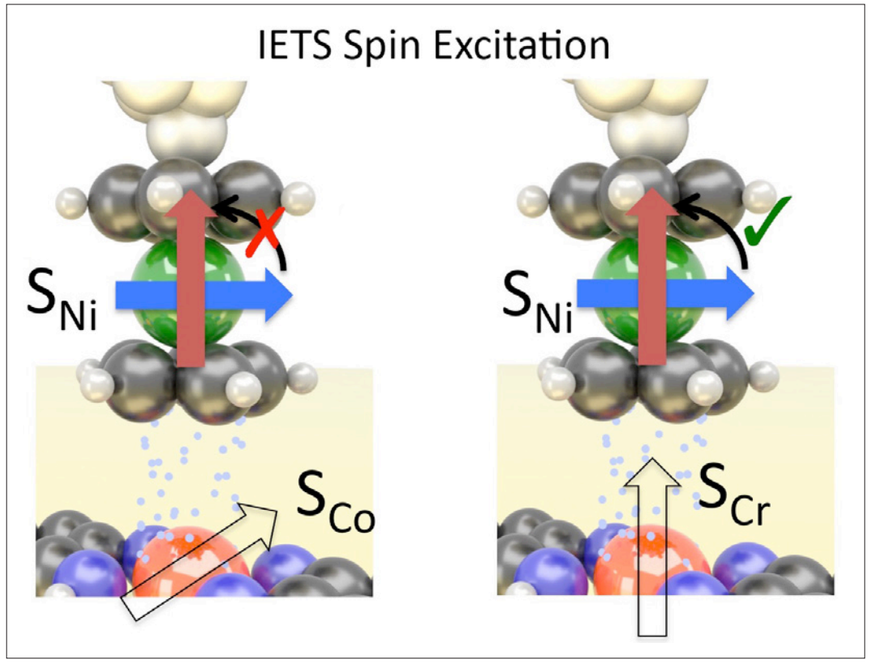
Wackerlin C, Cahlik A, Goikoetxea J, Stetsovych O, Medvedeva D, Redondo J, Svec M, Delley B, Ondracek M, Pinar A, Blanco-Rey M, Kolorenc J, Arnau A, and Jelinek P
ACS Nano 16, 16402 (2022)

Understanding the basics of magnetism in low-dimensional systems represents a challenge from both fundamental and practical points of view. For example, according to the Mermin-Wagner theorem, magnetic order at finite temperatures can only be sustained in the presence of magnetic anisotropy in one- and two-dimensional systems. Additionally, since electron correlation effects are less screened in low dimensions, their description requires the use of a suitable methodology. Furthermore, from an experimental point of view, a detailed characterization of the electronic and magnetic properties requires the use of an ensemble of techniques, such as different X-ray absorption spectroscopies (XAS, XLD, XMCD), combined with local probe techniques, like inelastic electron tunneling spectroscopy.

Recently, it has been demonstrated [Angew. Chem., Int. Ed. 2021, 60, 439–445] that it is possible to synthetize rather long (> 100 nm) metal-organic coordination polymers by the reaction of transition metal atoms and organic molecules on a metal surface. On rather inert surfaces, like Au(111), the properties of the one-dimensional (1D) coordination polymers are essentially preserved, allowing to investigate their intrinsic properties. A significant breakthrough in the characterization of the magnetic properties of nanostructured surfaces has been the use functionalized STM tips with magnetic molecules, like nickelocene ($NiCp_2$) [Science 2019, 366, 623–627]. This permits to achieve atomic resolution while probing the magnetic coupling between the tip and the sample with high sensitivity.

In this work, Pavel Jelínek and coworkers have combined different methods to achieve a complete characterization of the magnetic properties of 1D metal-organic chains that contain Cr or Co magnetic atoms coordinated with the organic ligand 2,5-diamino-1,4-benzoquinonediimine(QDI). More specifically, they have determined: (i) the spin state of the magnetic atoms, finding a spin crossover transition in the Co case, (ii) the magnetic anisotropy, and (iii) the different couplings between the nickelocene tip and the two magnetic atoms. In this way, they have shown that inelastic electron tunneling spectroscopy acquired with nickelocene decorated tips, in combination with a proper methodology for its interpretation, is a formidable characterization tool for atomic spin sensing.

Functionalized STM tips allow characterization of single-atom magnetic properties



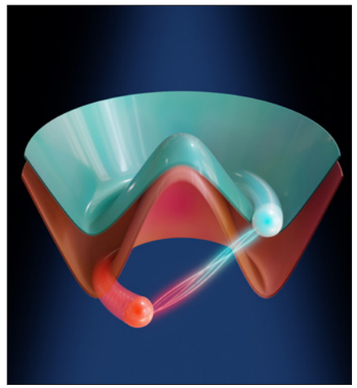
Nickelocene, in its excited state, shows perpendicular spin anisotropy (red arrow). Using the exchange coupling of the Ni spin with the Cr and Co single spins, we can characterize the magnitude and anisotropy by inelastic tunneling spectroscopy. The spin excitations that appear in the differential conductance are modulated by the relative orientation of both spins. In the case of CrQDI, the parallel alignment of spins gives rise to the splitting of the main peak associated to the Ni spin excitation, while for CoQDI the perpendicular alignment suppresses the exchange coupling between Ni and Co spins and only one peak is observed.

DIPC HIGHLIGHT 2022

Observation of superconducting collective modes from competing pairing instabilities in single-layer $NbSe_2$

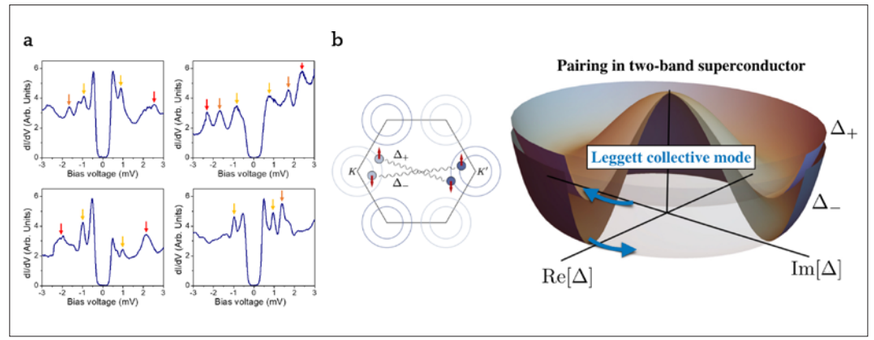
Wan W, Dreher P, Munoz-Segovia D, Harsh R, Guo HJ, Martinez-Galera AJ, Guinea F, de Juan F, and Ugeda MM
Advanced Materials 34, 202206078 (2022)

"Unconventional superconductivity" is a catch-all term that applies to multiple forms of superconductivity that deviate from the paradigm of BCS theory (=Cooper pairing in a spin-singlet, s-wave channel mediated by phonons). Layered materials (from cuprate oxides to twisted devices) are particularly appealing in this context, especially in the two-dimensional limit due to the reduced screening of electron interactions, which can lead to competing phases. Writing in Advance Materials, Wen Wan, Paul Dreher, and Rishav Harsh in the group of Miguel Ugeda at DIPC have reported the experimental observation of superconducting collective modes in a single layer of $NbSe_2$ that are in fact the result of the competition between pairing instabilities in different symmetry channels.



This material develops a charge density wave (CDW), and even at lower temperatures the material becomes a superconductor which survives down to the single-layer limit. Miguel and his team observed signatures of both phenomena by means of scanning tunneling spectroscopy in a monolayer of $NbSe_2$: first a soft gap corresponding to a CDW that only gaps a fraction of the Fermi surface, and then a sharp U-shape gap at T = 0.34 K flanked by coherence peaks.

However, the most striking observation was the systematic appearance of dip-hump features both in the electron and hole sides of the spectra taken, see panel a of the figure. Interestingly, these features were found equidistant in energy. The main energy values of the identified dip-hump features (as defined from the nearest coherence peak) appear to be in all cases multiple of the energy of the first peak, which led the authors to interpret them as harmonics of a fundamental mode. Lastly, these satellite peaks disappear along with the superconductivity when the temperature was raised or a magnetic field was applied. The energy of the fundamental mode was always smaller than the pair-breaking scale set by the superconducting gap.



Leggett modes in single-layer $NbSe_2$. (a) Four representative spectra acquired at T=0.34K. The yellow arrows identify the fundamental mode, the red arrows are the rest of harmonics. (b) Schematic representation of pairing in the Fermi surface consisting of two spin-polarized pockets around each valley. The collective mode corresponds to oscillations in the relative phase of the outer (+) and inner (-) pairing gaps.

The experimental observation of superconducting collective modes in a single layer of $NbSe_2$

With all this information the authors concluded that these features were the result of elastic quasiparticle scattering from a collective mode intrinsic to the superconducting state. But... what kind of collective mode? One possibility is the boson mediating the pairing interaction. But another possibility is some fluctuation in the particle-particle channel signaling the presence of a competing superconducting state. Daniel Munoz-Segovia with Fernando de Juan also at DIPC worked out a model favoring this latter scenario, which is natural in the context of this material. The model concerns only electrons at the two inequivalent corners (or valleys) of the hexagonal Brillouin zone. One can pair electrons from opposite valleys in different spin configurations with the only constraint of Pauli exclusion principle. In particular, one can form singlet s-wave and triplet f-wave pairings, and if interactions involving momentum exchanges between valleys were neglected, these two states would be degenerate. In reality this interaction is small (smaller than intra-valley interactions) but different from zero: one state wins, but there is a nearby saddle point in the free energy corresponding to the other possible solution. There is then the possibility of "oscillating" between these two states; the collective mode associated with this "oscillation" would be of the Bardasis-Schrieffer type. However, the situation is slightly different: the material is non-centrosymmetric and spin-orbit coupling is sizeable, which means that these two states can actually be admixed (they have the same symmetry under doubled point group operations). The situation is more akin to the multi-band scenario first envisioned by Leggett and illustrated in panel b of the figure: The collective mode is associated with the oscillations in the relative phase of the pairing in the inner and outer Fermi pockets.

These findings are not only relevant in the specific context of $NbSe_2$, where the competition with another spin-triplet nematic superconductor is possible, but in the broader context of other reports of superconductivity in two-dimensional hexagonal crystals, where the multi-valley character of the bands calls for competitions of similar nature.

DIPC HIGHLIGHT 2022

Near-unity triplet generation promoted via spiro-conjugation

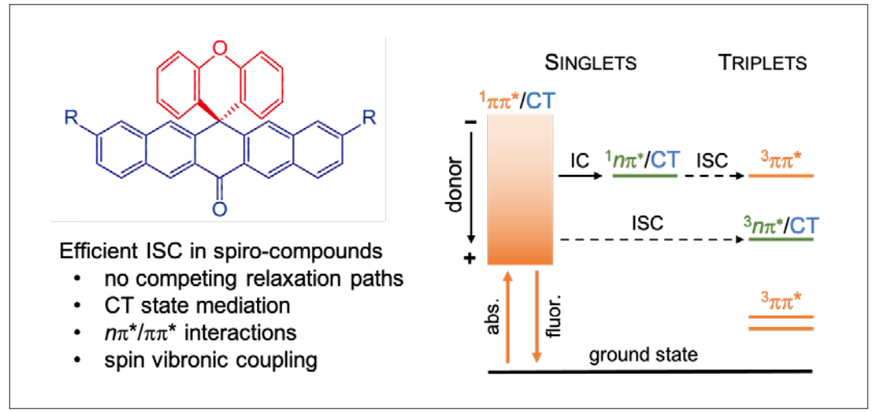
Lv M, Lu XC, Jiang YR, Sandoval-Salinas ME, Casanova D, Sun HT, Sun ZR, Xu JH, Yang YJ, and Chen JQ
Angewandte Chemie-International Edition 61, e202113190 (2022)

There is a process, called intersystem crossing, in which a singlet excited electronic state makes a transition to a triplet excited state at the point where the potential energy curves for the excited singlet and triplet states cross. Importantly, this transition is forbidden in the absence of spin-orbit coupling but occurs in the presence of spin-orbit-coupling. This is why several structural features often lead to triplet state generation in organic chromophores. For example, the incorporation of heavy-atoms facilities intersystem crossing through an enhanced spin–orbit coupling. A triplet formed via intersystem crossing is frequently in an excited vibrational state.

Interestingly, charge recombination due to a charge transfer also results in an efficient triplet state generation, in which the orbital angular momentum change induced by the charge recombination is compensated by a spin flip for total angular momentum conservation. This mechanism, referred to as spin–orbit charge transfer intersystem crossing (SOCT-ISC), has led to the discovery of a range of triplet sensitizers.

But it is not that easy. The excited vibrational triplet state can reach its lowest vibrational state by collisions with other molecules. The transition from this state to the singlet state is forbidden in the absence of spin-orbit coupling but allowed when there is spin-orbit coupling. This gives rise to the slow emission of electromagnetic radiation known as fluorescence. Given that fluorescence emission, vibrational relaxation or charge recombination directly to the ground state, usually co-exist with intersystem crossing, it is rather difficult to manipulate these processes through chemical modification. Multiple factors enhancing intersystem crossing interfere with each other and, in order to maximize triplet yield, other competitive excited state relaxation channels have to be suppressed. So, it comes as no surprise that these exceptional collection of features in a molecule is rarely reported.

A spiro compound is a molecule in which there are two rings linked through a single atom (the spiro atom). A team of researchers had shown that the use of a spiro-linkage can lock the electron donor and acceptor in an orthogonal geometry with close proximity Now, that same team reports 1 the synthesis and photophysical properties of a family of spiro-conjugated triplet generators in solution.



Efficient ISC in spiro-compounds mediated by charge-transfer, nπ*/ππ* interactions and spin vibronic coupling results in ~100% triplet state generation.

Multiple important factors can be combined to enhance triplet state generation without interference via a rigid asymmetric spiro-conjugated molecular motif

Intersystem crossing is enhanced so much in spirobis[anthracene]-diones, that a record-high SOCT-ISC rate constant is achieved. This rate constant is inherited by the new spiro-conjugated triplet generators due to their asymmetry. Triplet generation efficiency could be further enhanced by stabilizing the spiro-charge-transfer state. The new spiro-compounds consist of electron-rich diphenyl ether as the donor and electron-deficient dinaphthyl ketone as the acceptor. Through side group engineering, near-unity triplet generation is achieved with further assistance from spin-vibronic coupling.

The application of the new compounds as triplet sensitizers and in medicine was tested by triplet-triplet energy transfer and photodynamic therapy experiments. These results show that multiple important factors can be combined to enhance triplet state generation without interference via a rigid asymmetric spiro-conjugated molecular motif, providing a pathway to the design of heavy-atom-free triplet sensitizers with predictable properties.

DIPC HIGHLIGHT 2022

Hydrogen tunneling in catalytic hydrolysis and alcoholysis of silanes

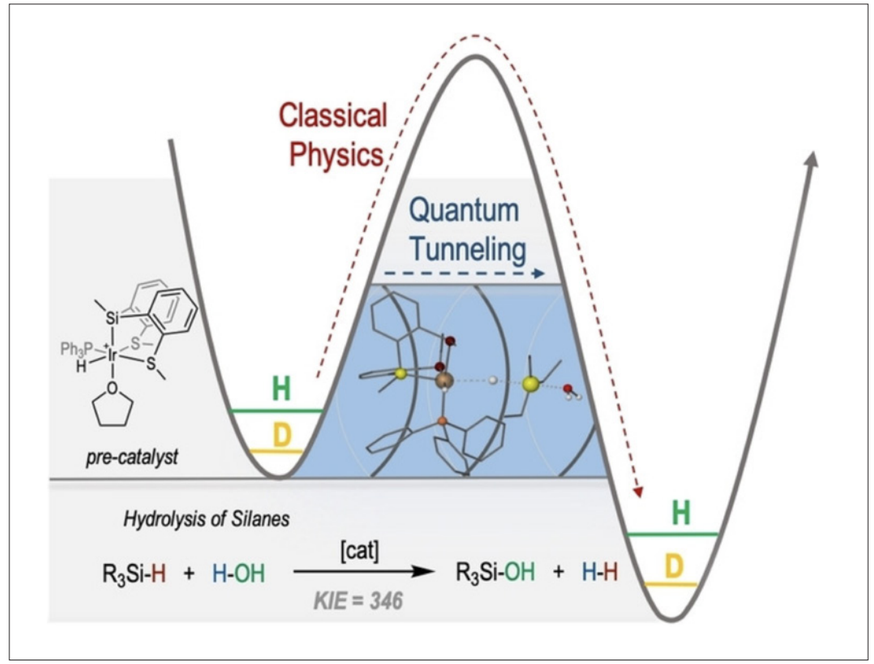
Almenara N, Garralda MA, Lopez X, Matxain JM, Freixa Z, and Huertos MA
Angewandte Chemie-International Edition 61, e202204558 (2022)

The unprecedented challenges faced by our society in terms of energy production and consumption have stimulated considerable efforts by the scientific community to develop new energy sources. Among the possible alternatives to fossil fuel resources, hydrogen stands out as a promising candidate. Recently, hydrolysis and alcoholysis of hydrosilanes have received much attention as a possible source for hydrogen. To overcome the slow kinetics of these reactions, transition metal-based catalysts are used, with cationic iridium species showing the best performances so far. Assuming an electrophilic mechanism for the hydrolysis/alcoholysis of silanes that was proposed in the late 90s, several studies have been reported for systems involving different transition metals, all relying on "classical" reaction routes.

In this paper, scientists from DIPC and UPV/EHU report for the first time the case of hydrosilane activation with the participation of quantum tunneling. Combining experimental evidences and detailed DFT calculations, they demonstrate the importance of hydrogen quantum tunneling in the efficiency of the cationic hybrido-silyl-IrIII complex as a precatalyst for the hydrolysis/alcoholysis of tertiary silanes.

Kinetic Isotopic Effect (KIE), which has a typical value of around 1-8 when tunneling effects are negligible, is computed as the ratio between the measured rate constants for H and D, respectively, kSi-H/kSi-D. In the case of HSiEt3 and DSiEt3, assisted by the catalyst mentioned above, the KIE value was measured to be 346, which represents the largest value involving Si–H/D bonds observed up to date. Other experimental evidences of the importance of hydrogen quantum tunneling in the Rate Determining Step (RDS) of this reaction were the calculated Arrhenius factor, the difference in the observed activation energy and the temperature dependence of the KIE. In order to understand these experimental evidences, DFT calculations were carried out first to characterize the reaction mechanism and to quantify the tunneling effects in the RDS. These calculations on the reaction mechanism propose a slightly modified electrophilic mechanism for the reaction compared to the previously reported ones. In addition to this, quantum tunneling effects were computed by means of the qualitative WKB one-dimensional tunneling correction. These calculations were able to predict the KIE behavior with the temperature, and support the importance of quantum tunneling.

A fast and green catalytical chemical reaction for hydrogen production based on the hydrolysis of silanes



An unprecedented quantum tunneling effect has been observed in catalytic Si–H bond activations at room temperature.

The nature of the iridium catalyst with a silicon atom in trans position is critical to provoke the hydride tunneling and accelerate the reaction

DIPC HIGHLIGHT 2022

Metal substrate catalysis in the confined space for platinum drug delivery

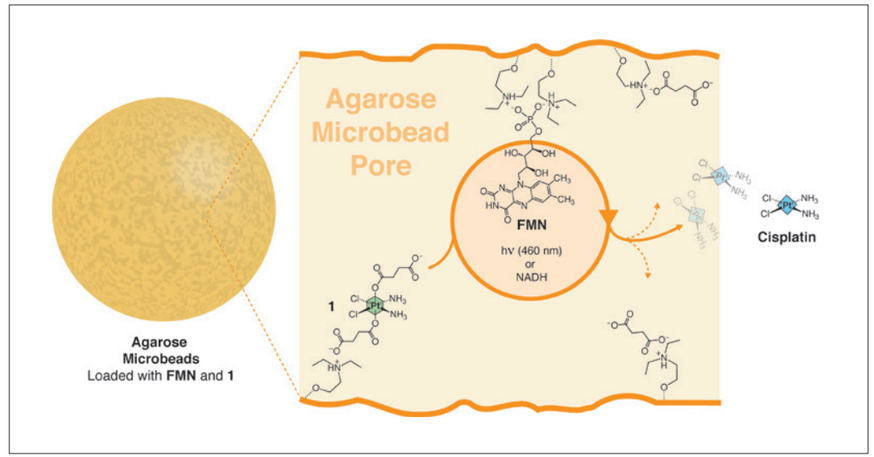
Velasco-Lozano S, Alonso-de Castro S, Sanchez-Cano C, Benitez-Mateos AI, Lopez-Gallego F, and Salassa L
Chemical Science 13, 59 (2022)

Metal complexes, artificial metalloenzymes and nanomaterials can catalyse abiotic reactions in biological environments, both in vitro and in vivo. In the context of chemotherapy, metal complexes have been designed to function as catalysts for the deprotection of organic anticancer agents and for the oxidation/reduction of biomolecules that are key for the cell homeostasis. Something similar happens with metal-loaded catalytic nanocarriers, that have been engineered to be delivered to tumours, or to be placed in their proximity during a surgical procedure, where they can trigger the conversion of prodrugs into their biologically active counterparts.

The great majority of the schemes proposed so far display rather modest catalytic efficiencies, even in buffer solutions, as evidenced by low turnover numbers and slow reaction kinetics. The kinetic aspect is especially overlooked, in spite of its key importance in the development of drug activation strategies. With few exceptions, catalysts currently known typically achieve substrate conversion rates in solution that are in the order of 10-3 to 10-1 min-1. This means that almost any benefit is lost, as this low turnover frequency implies long exposure periods or high loads in order to transform enough prodrug into active drug to induce the desired therapeutic effects. If we now consider the catalyst intrinsic toxicity and that the choice of drugs with high-potency often becomes mandatory, the net result is a limitation in the therapeutic use of catalysis-based strategies.

Flavins and selected flavoproteins photocatalytically convert Pt(IV) prodrug precursors into clinically-approved cisplatin and carboplatin with high efficiency, showing a turnover frequency 25 min-1. Given the exceptional anticancer activity of Pt chemotherapeutics the team speculated that the catalytic efficiency of these flavin-mediated reactions could be the base for a convenient solution for the administration of cisplatin and its derivatives.

The researchers sought inspiration in nature, which confines biocatalysts (enzymes) and substrates (metabolites) inside organelles to control biosynthetic pathways and boost catalytic performance. This is not new, though, after all, catalysts confined into supramolecular structures have proved very effective in favouring chemical reactions for different technological purposes. However, none of the state-of-the-art systems involve confinement of the catalyst and its corresponding prodrug substrate into an artificial chassis that can operate as a drug depot.



Flavin-catalyzed generation of cisplatin from a Pt(IV) prodrug precursor inside diethylaminoethyl agarose microbeads (AGM).

Flavin-based catalytic hydrogels for the delivery of anticancer platinum drugs

Hydrogels have been widely used as solid supports to immobilize different types of catalysts. These biocompatible soft materials can be applied in surgical implants, locally injected or administered systematically via intravenous infusion, or used to fabricate therapeutic patches for intra- and transdermal release of pharmaceuticals. Stimuli responsive hydrogels introduce an additional level of control on the drug action.

The researchers show how loading of a Pt(IV) prodrug complex and a flavin catalyst onto a hydrogel (agarose porous microbeads) enables performing in situ the confined catalytically-driven generation and subsequent release of cisplatin in response to stimuli, both light and chemical activation. This is a different approach from the usual, where catalysis has so far been employed to accelerate the degradation of hydrogels and thus control the delivery of the active agents, rather than activating a confined prodrug.

These results may provide a general method to produce remote-controlled high local concentrations of Pt drugs in short bursts. In the long run, this could represent a viable strategy to develop topical medicaments and implantable devices that may overcome some issues associated with the systemic administration of Pt chemotherapeutic agents.

DIPC HIGHLIGHT 2022

Theoretical studies of furan and thiophene nanothreads: structures, cycloaddition barriers, and activation volumes

Chen B, Crespi VH, and Hoffmann R
Journal of the American Chemical Society 144, 9044 (2022)

Nanothreads are one-dimensional nanomaterials composed of a primarily sp3 hydrocarbon backbone, typically formed through the compression of small molecules to high pressures. A defining feature of nanothreads is their unique combination of extreme thinness (only a few angstroms in diameter) and rigidity (multiple single covalent bonds connecting each unit). This feature distinguishes nanothreads both from traditional polymers, which are generally flexible (by rotation around single bonds), and from nanotubes or nanowires, which are normally much thicker.

Rigidity is a defining property of hard (not soft) condensed matter; when accompanied by periodicity (for which it is a precondition), it is intimately associated with a manifold of condensed-phase properties. Nanothreads were first synthesized from benzene under pressure in diamond anvil cells or Paris–Edinburgh cells, but the high-pressure solid-state synthesis technique appears to be quite general for unsaturated hydrocarbons. Whereas previous high-pressure reactions of small molecules resulted in amorphous products, the discovery of ordered nanothreads hints at the possibility of rational design principles for the controlled formation of crystalline extended solids at high pressure. Thus, combining physical rigidity with chemical kinetic control, one could design nanothread precursors that capture and recover molecular orbital alignments, so long as the ligands in question can be anchored to the thread backbone.

Interestingly, when precursors contain a heteroatom, as in two aromatics similar in structure, furan (a ring consisting of four CH groups and one oxygen atom) and thiophene (a ring of four CH groups and one sulphur atom), the nanothreads show enhanced structural order due, in large part, to their localized bonding. Furan and thiophene were shown to form nanothreads at 15 and 35 GPa, respectively. Now, a team of researchers theoretically examines the formation, structure, and stability of these two nanothreads, the most ordered ones produced yet (Figure 1).

The researchers examine three main themes. First, understanding the 20 GPa difference in the synthetic pressure (both the onset and maximum pressures) in the two nanothread syntheses. They find that the difference is explainable in terms of the greater loss of aromaticity by the thiophene.

Next, they focus on the effect of pressure on these cycloadditions using the recently developed Cammi's extreme pressure polarizable continuum model (XP-PCM) methodology. The computed high-pressure reaction profiles of five representative reactions of the [4 + 2] polymerization show that pressure decreases the reaction barriers of all these cycloadditions due to the volume reduction nature of these bond-forming cycloadditions.

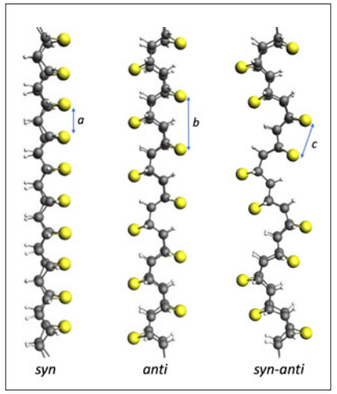


Figure 1. Three characteristic furan or thiophene nanothread structures, in idealized form. Carbons in grey, hydrogens in white, and chalcogens (O or S) in yellow. In the DFT-relaxed (using the PBE functional) structures, a = 2.6 Å, b = 4.6 Å, and c = 2.8 Å for furan threads, and a = 2.8 Å, b = 4.7 Å, and c = 3.2 Å for thiophene threads.

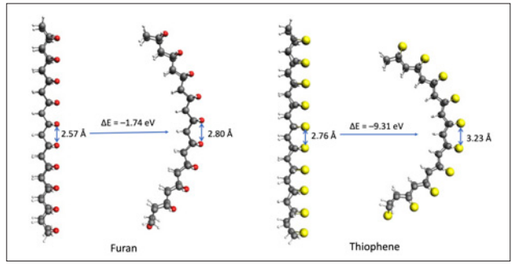


Figure 2. Structural and energy changes upon relaxation of two 10-unit segments of the straight syn threads of furan and thiophene, calculated at the PBE-D3BJ/6-31G(d) level of theory.

A defining feature of nanothreads is their unique combination of extreme thinness (only a few Å in diameter) and rigidity (multiple single covalent bonds connecting each unit)

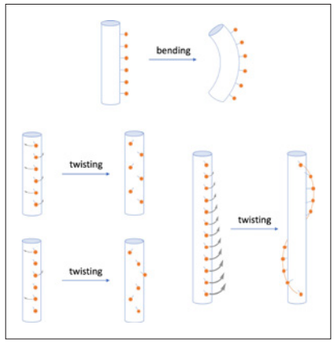


Figure 3. Illustration of thread bending (arching) and twisting as results of axial and lateral relaxations of the lone pair repulsion between the chalcogens (orange balls) in the syn thread.

Finally, the team goes on to rationalize the structures and relative stabilities of the syn, syn–anti, and anti furan/thiophene nanothreads formed from [4 + 2] cycloaddition pathways. The syn polymer, with all O/S atoms on the same side, if not allowed to distort, is at a high energy relative to the other two due to the O/S lone pair repulsion, understandably greater for S than for O at the 2.8/2.6 Å separation (Figure 2). Set free, the syn isomers curve or arch in two- or three-dimensional (helical) ways, whose energetics are traced in detail (Figure 3). The syn polymer can also stabilize itself by twisting into zig-zag or helical energy minima. The release of strain in a linear thread as the pressure is relaxed to 1 atm, with consequent thread curving, is a likely mechanism for the observed loss of the crystalline order in the polymer as it is returned to ambient pressure.

This work provides a reasonable understanding of the factors, both intrinsic and comparative, that govern ideal furan and thiophene nanothreads. This knowledge will inform the consideration of the possibilities for other nanothreads as well.

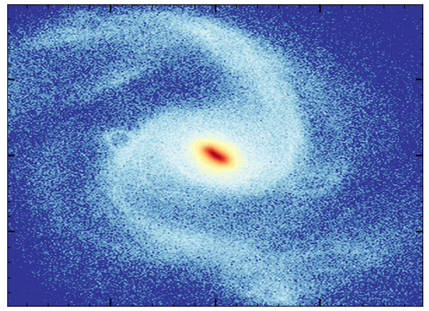
DIPC HIGHLIGHT 2022

Disc instability and bar formation: view from the IllustrisTNG simulations

Izquierdo-Villalba D, Bonoli S, Rosas-Guevara Y, Springel V, White SDM, Zana T, Dotti M, Spinoso D, Bonetti M, and Lupi A
Monthly Notices of the Royal Astronomical Society 514, 1006 (2022)

Barred galaxies are spiral galaxies characterized by a prominent bar-shaped structure at their center. These structures are composed of stars, whose orbits give rise to these peculiar shapes. Our own galaxy, the Milky Way, has a bar at its center.

The large majority of spiral galaxies is barred, thus understanding how these structures form and affect the evolution of the full galaxy is important for a global understanding of galaxy evolution.



Rosas-Guevara et al. 2022

A2_099: An example of a barred galaxy in the TNG50 simulation. The image is a density map of simulated stars.

In this paper, co-authored by the DIPC researchers Silvia Bonoli, Ikerbasque Research fellow, and Yetli Rosas Guevara, Juan de la Cierva senior postdoc, the team investigates the physical properties and environment of the galaxies in which these structures are born, using the simulated barred galaxy sample extracted from two state-of-the-art hydrodynamical cosmological simulations, the TNG100 and TNG50 (https://www.tng-project.org/). The authors find that most bar structures form in galaxies whose disk component is predominant with respect to other components, as previously speculated on more simplified simulations. Moreover, they report that galaxies that form a bar assembled earlier in the history of the universe, and have a stellar content which is very concentrated. They also find that, while the majority of bar structures develop in galaxies in isolation, a small fraction of bars seems to develop in galaxies which are disturbed by a close companion. In the future, the team will further investigate how star formation in galaxies is affected by the presence of these structures and how bars can help "feeding" the supermassive black holes which are located at the centers of all galaxies.

Understanding how these structures form and affect the evolution of the full galaxy is important for a global understanding of galaxy evolution

NASA, ESA and The Hubble Heritage Team (STScI/AURA)

Hubble: NGC1300, a typical example of a barred spiral galaxy.

DIPC HIGHLIGHT 2022

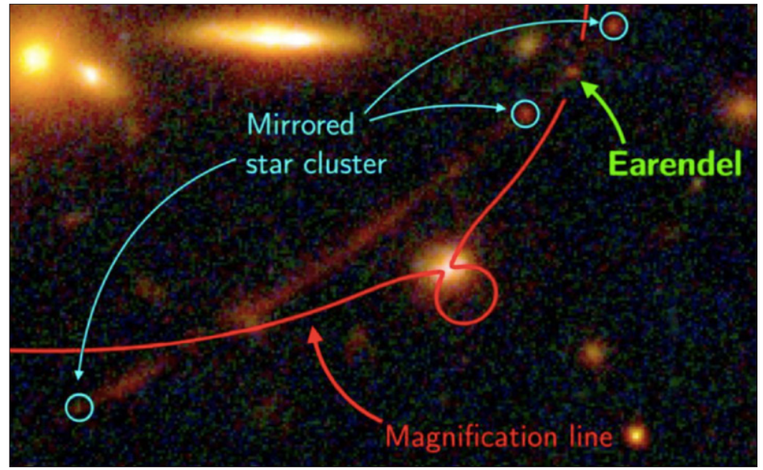
A highly magnified star at redshift 6.2

Welch B, Coe D, Diego JM, Zitrin A, Zackrisson E, Dimauro P, Jimenez-Teja Y, Kelly P, Mahler G, Oguri M, Timmes FX, Windhorst R, Florian M, de Mink SE, Avila RJ, Anderson J, Bradley L, Sharon K, Vikaeus A, McCandliss S, Bradac M, Rigby J, Frye B, Toft S, Strait V, Trenti M, Sharma S, Andrade-Santos F, and Broadhurst T
Nature 603, 815 (2022)

A gravitational lens is any object that deflects light by gravitation as described by the general theory of relativity; it is analogous to a lens in optics. This includes the biggest lenses in in the universe, galaxy clusters where the magnification can be as high as tens or hundreds, stretching galaxies into giant arcs, and in the case of the newly discovered Individual stars detected by Hubble even higher magnification is attained given fortuitous alignment with the lensing cluster.

A team using the Hubble Space Telescope, including Tom Broadhurst at the DIPC, has now used gravitational lensing to discover distant stars lensed by the most massive galaxy clusters, finding the most distant known star within a high redshift galaxy that dates to just 900 million years after the Big Bang. This star is magnified by a factor of thousands by a foreground galaxy cluster lens called WHL0137–08 (redshift 0.566) as shown in the figure here. This star they have named "Earendel" meaning "morning star" in old English, because of its appearance when the Universe was young and stars and galaxies were forming for the first time. The figure also shows how the host galaxy of this star is spread out into a giant "arc" by the lensing effect of the galaxy cluster - much like the lensing effect of looking through the base of a wine glass.

Four different lensing models built by the astronomers lead to the conclusion that we are seeing here a single star (or a binary) of mass greater than 50 times the mass of the Sun that is fortuitously located right on the Einstein ring of this lens (denoted "Magnification line" in figure), and thus receiving an enormous magnification that allows ditch a distant star to be detected by Hubble. The spectral type, temperature and mass of the star remain uncertain. Future spectroscopic observations with James Webb Spatial Telescope are now ongoing to establish its properties more accurately and to find many more such stars that will allow us to chart more fully the evolution of star formation over the course of cosmic history.



Hubble telescope image of a galaxy forming a giant red arc of a background galaxy that is lensed by the gravity of a foregrund cluster or galaxies, much like the lensing effect of looking through the base of a wine glass. Within this lensed galaxy is a star magnified by a factor of thousands by a foreground galaxy cluster lens we named "Earendel" meaning fortunately located right on the Einstein ring of this lens-denoted by the red "Magnification line" shown, and thus receiving an enormous magnification that allows such a distant star to be detected here by Hubble.

The most distant star seen through a "cosmic wine glass"

This discovery builds on the first discovery by the Hubble "Flashlights" team that Tom Broadhurst as a founding member recognised that a mysterious "transient" point source rose and faded near the Einstein ring of another massive galaxy cluster, was in fact an individual bright star lensed by the cluster. This star was named Icarus and published in Nature Astronomy in 2015 with his colleagues. Since then several similar examples have been found with Earendel being the most distant example and readily detected by the James Webb Telescope. This new star lensing phenomenon will provide a steady increase in our understanding of the hot young stars formed in the early Universe.

DIPC HIGHLIGHT 2022

Switchable chiral transport in charge-ordered Kagome metal CsV_3Sb_5

Guo CY, Putzke C, Konyzheva S, Huang XW, Gutierrez-Amigo M, Errea I, Chen D, Vergniory MG, Felser C, Fischer MH , Neupert T, and Moll PJW
Nature 611, 461 (2022)

Chiral matter offers opportunities for the exquisite control of electron and spin transport due to extraordinary optical, electronic, and magnetic properties that depend on the structure's handedness. Importantly, these properties are often observed at or near room temperature, which suggests that quantum devices based on chiral matter and fields have the potential to operate at similar practical temperatures if properly designed.

Crystals are structurally chiral if they possess no mirror, inversion or roto-inversion symmetry, giving rise to left- and right-handed enantiomers. This chirality can be imprinted on the crystals' emergent excitations, which are then also characterized by a definite handedness. The interaction between structural chirality and the breaking of time-reversal symmetry is of particular interest, as it links the static chirality to temporal processes, such as growth, catalysis and wave propagation. Response functions that jointly arise because of chirality and time-reversal symmetry breaking arecalled magnetochiral anisotropies.

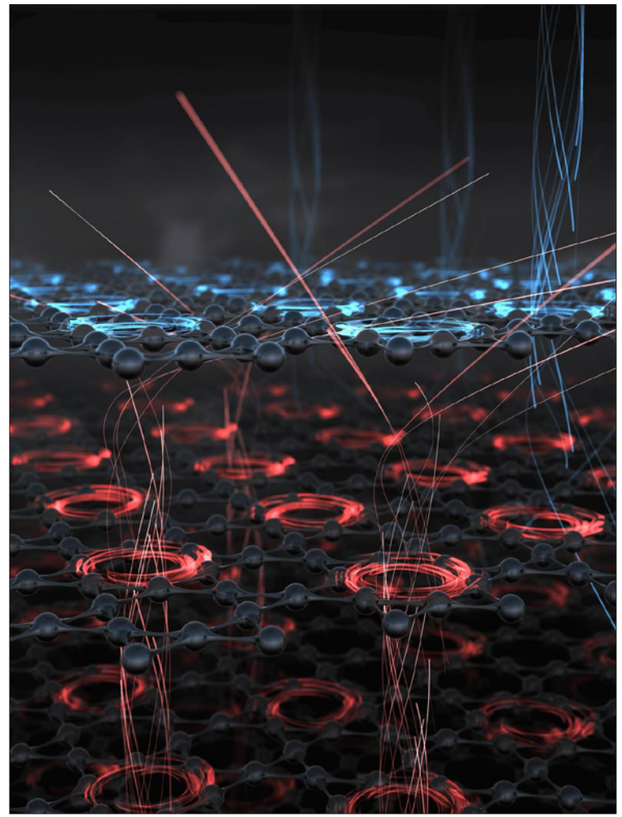
Specifically, in metals, electronic magnetochiral anisotropy (EMA) —a change in resistance due to an applied current and an external magnetic field— opens up possibilities to detect, manipulate and utilize chiral properties in electronics.

In order to display EMA, a conductor must break inversion symmetry, which can occur as a weak effect in any metal when its macroscopic shape is chiral, for example, in a coil. Alternatively, materials with chiral crystal structure generally show EMA in any conductor shape.

EMA expresses an imbalance between scattering processes of different handedness, which can occur either from the intrinsic handedness of the carriers in chiral crystals, or extrinsically from chiral defects, as in plastically twisted conductors. When electronic interactions form ordered phases within chiral materials, as, for example, in chiral magnets, EMA can be further amplified via scattering off, for example, an emergent chiral spin texture.

Now, a team of researchers demonstrates 1 EMA in a rectangular bar of centrosymmetric CsV_3Sb_5, a layered metal in which vanadium atoms form kagome nets. Chiral transport is observed via second-harmonic generation under an in-plane magnetic field.

The EMA signal becomes significant only at temperatures below 35 K, deep within the charge-ordered state of CsV_3Sb_5 (94 K). This temperature dependence reveals a direct correspondence between electronic chirality, unidirectional charge order and spontaneous time-reversal symmetry breaking due to putative orbital loop currents.



Chiral electronic transport in the CsV_3Sb_5 metal.

The measured chiral electronic transport in this work adds up to list of unconventional properties of the Kagome CsV_3Sb_5 metal

The researchers show that the chirality is set by the out-of-plane field component, and that a transition from left- to right-handed transport can be induced by changing the field sign. CsV_3Sb_5 is the first material in which strong chiral transport can be controlled and switched by small magnetic field changes, in stark contrast to structurally chiral materials, which is a prerequisite for applications in chiral electronics.

Although the small absolute magnitude and extreme environmental conditions probably preclude direct applications of CsV_3Sb_5, these results showcase that spontaneous symmetry breaking can be used to transform small changes in external fields into singular changes in the response functions of chiral conductors.

DIPC HIGHLIGHT 2022

Circumventing the stability problems of graphene nanoribbon zigzag edges

Lawrence J, Berdonces-Layunta A, Edalatmanesh S, Castro-Esteban J, Wang T, Jimenez-Martin A, de la Torre B, Castrillo-Bodero R, Angulo-Portugal P, Mohammed MSG, Matej A, Vilas-Varela M, Schiller F, Corso M, Jelinek P, Pena D, and de Oteyza DG
Nature Chemistry 14, 1451 (2022)

In the last decades, a new synthetic approach has been developed, generally termed as "on-surface synthesis" that substantially departs from standard chemistry in solution. Instead of the three-dimensional space of solvents in the latter, the environment of the reactants in this new approach are well-defined two-dimensional solid surfaces that are typically held under vacuum conditions.

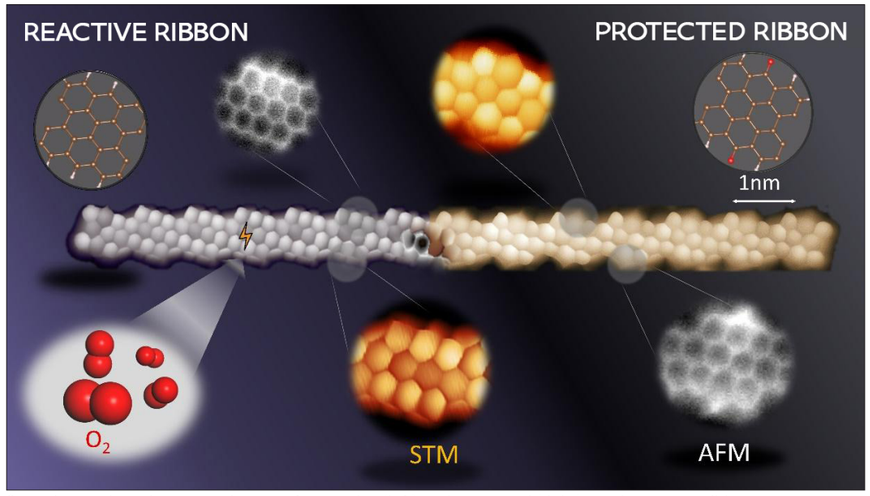
These differences have allowed the successful synthesis of a great variety of molecular structures that could not be obtained by conventional means. Among the structures that are raising particular interest, we find carbon-nanostructures with zigzag-shaped edges, which endow the materials with exciting electronic and even magnetic properties of potential interest for a great variety of applications that include quantum technologies.

An important downside of these materials, however, is that they often lack sufficient chemical stability to withstand air exposure. That is why environments like vacuum are used to make the synthesis possible. Unfortunately, for their ultimate implementation in actual devices, these structures need to be manipulated and transferred out of the vacuum, which would degrade the materials and therefore jeopardize their potential utilization. This brings up the need to conceive new strategies for the device fabrication processes.

In conventional chemistry, protection/deprotection strategies are commonly applied to overcome stability problems. However, it remained to be tested whether such protection chemistry strategies could also be applied in "on-surface synthesis". Now, a team of researchers has performed such tests with narrow stripes of graphene nanoribbons featuring a large density of zigzag-shaped edges. The work presents two related but complementary methods to apply the protection/deprotection strategy to the reactive zigzag edge segments of nanographenes.

In particular, they have demonstrated the usage of atomic hydrogen as a means of protecting the nanostructured graphene from the oxidising effects of the atmosphere. Afterwards, the nanostructures were easily dehydrogenated and converted back to their original form via annealing. An alternative approach further allowed them to convert an air-stable, chemically modified form of the graphene nanostructures with protective ketone side groups, into the molecules of interest.

A breakthrough towards the integration of chemically labile carbon nanostructures into devices



Scanning probe microscopy image of a reactive (left) and protected (right) graphene nanoribbon.

They have demonstrated the usage of atomic hydrogen as a means of protecting the nanostructured graphene

The implications of these results are far-reaching. The demonstrated protection/deprotection strategy is expected to be similarly applicable to graphene nanostructures with zigzag edge segments different from those probed here. It thus opens new doors for the conception of approaches to integrate carbon nanostructures into devices and may thereby bring the exploitation of the unique characteristics of their zigzag edges a step closer to scalable applications, a grand scientific challenge that cuts across physics, chemistry, materials science and engineering.

DIPC HIGHLIGHT 2022

Superconducting spintronic tunnel diode

Strambini E, Spies M, Ligato N, Ilic S, Rouco M, Gonzalez-Orellana C, Ilyn M, Rogero C, Bergeret FS, Moodera JS, Virtanen P, Heikkila TT, and Giazotto F
Nature Communications 13, 2431 (2022)

Patent: Apparatus and Method for Superconducting Diode
Inventors: Ilic S, Bergeret FS, Giazotto F, Strambini E, Spies M, Virtanen P, and Heikkilä TT
Application PCT/IT21/000038 filled in 23/07/2021

Diodes are essential in nowadays electronics as they allow current to flow in one direction. However, semiconductors have limitations at sub-Kelvin temperatures, which are crucial for cryogenic electronics and ultrasensitive detection.

Superconductors would be ideal candidates for the realization of cryogenic diodes and detectors due to their intrinsically low impedance, and the lower energy scales of the superconducting gap (~meV) compared to semiconductors (~eV). Still, the implementation of a superconducting diode turns out to be difficult since it requires breaking of the electron-hole symmetry, whereas the BCS superconducting state is, by definition, electron-hole symmetric.

To overcome this issue, the groups led by Celia Rogero and Sebastian Bergeret (Material Physics Center and DIPC), in collaboration with groups in Finland, Italy, designed and fabricated a new type of superconducting diode. It consists of a thin superconducting layer with an intrinsic spin-splitting field attached to an electrode via a spin-selective barrier, which breaks the electron-hole symmetry and makes the transport direction-selective. Two different types of diodes were fabricated based on the combination of the ferromagnetic insulator EuS and Al as a superconductor. The direction-selective propagation of the charge is obtained through the spin-selective barrier that can be achieved either through the EuS in a Al/EuS/Cu configuration or using a metallic ferromagnet as electrode in a EuS/Al/Co combination.

These junction achieve a large rectification (up to ~40%) already for a small voltage bias (~200 μV) thanks to the small energy scale of the system: the Al superconducting gap. Both theory and experiment confirmed that the maximum rectification of this cryogenic spintronic rectifier can be linked to the spin polarization of the barrier and exhibit quasi-ideal Shockley-diode behavior.

This innovative device has great potential for highly-sensitive radiation detection and may pave the way for low-dissipation and fast superconducting electronics.

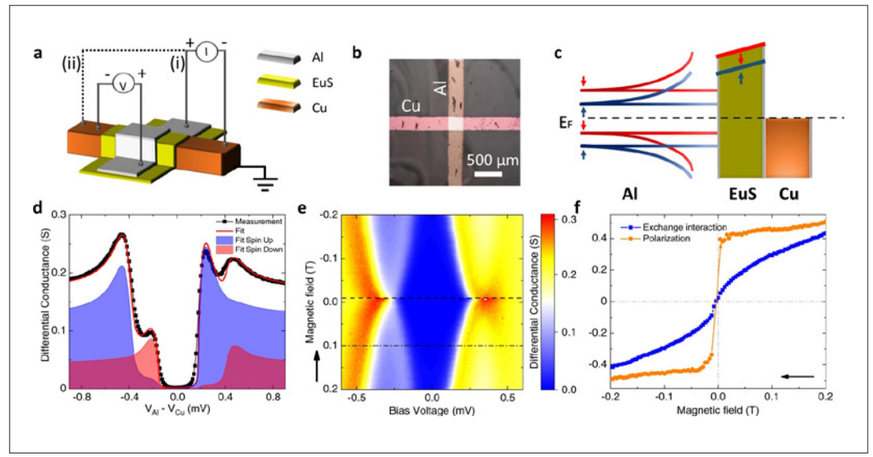


Figure 1: Working principle and characteristics of the superconducting tunnel diode: (a) Schematic of the device structure, (b) Visible light microscopy image of the device, (c) Schematic of the DoS, (d-f) Examples of results such as differential conductance curve (d), differential conductance color maps (e) and Exchange field (f).

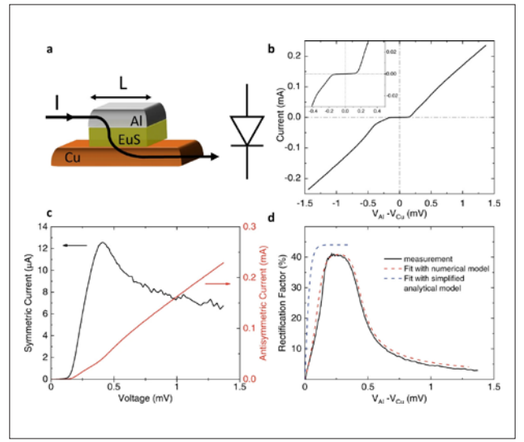


Figure 2: Rectification of the superconducting tunnel diode: a Schematic of the N/FI/S tunnel junction, b Current-to-Voltage (I(V)) characteristic, c Symmetric and antisymmetric parts of the I(V) characteristic, d Rectification coefficient.

A team of DIPC researchers developed a new type of superconducting diode to address the limitations of semiconductors at sub-Kelvin temperatures

DIPC HIGHLIGHT 2022

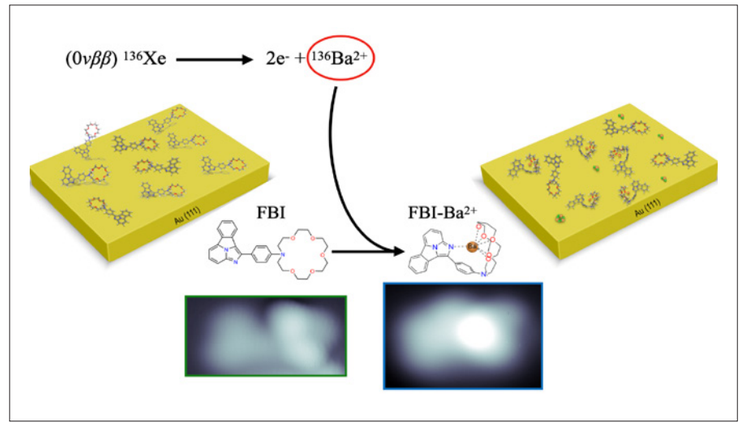
Ba^{+2} ion trapping using organic submonolayer for ultra-low background neutrinoless double beta detector

Herrero-Gomez P, Calupitan JP, Ilyn M, Berdonces-Layunta A, Wang T, de Oteyza DG, Corso M, Gonzalez-Moreno R, Rivilla I, Aparicio B, Aranburu AI, Freixa Z, Monrabal F, Cossio FP, Gomez-Cadenas JJ, Rogero C, and NEXT collaboration
Nature Communications 13, 7741 (2022)

Are neutrinos their own antiparticle? The NEXT collaboration is trying to answer this question by searching for the elusive nuclear reaction known as neutrinoless double beta decay. If this reaction takes place, it would prove the Majorana nature of neutrinos, and answer "yes" to this question. However, the lifetime expected for this process is in the order of 1027-1028 years, so the backgrounds must be suppressed to practically zero level. The neutrinoless double beta decay of ^{136}Xe produces a $^{136}Ba^{2+}$ dication and two electrons. If these products can be detected in delayed coincidence, it would unambiguously prove the occurrence of this extraordinary reaction. This is precisely what the NEXT collaboration proposes to do.

The experiment can already detect the two electrons and measure its energy, so the focus is now on the daughter dication. Finding a single Ba ion in a chamber containing around one tonne of xenon is a daunting task, but appears feasible thanks to fluorescent organic molecules designed specifically to capture barium. The ion will drift in an electric field inside the NEXT chamber toward a monolayer of molecules, will be captured by one, which will thereby change their optical properties. This is the working principle of so-called Fluorescence Bicolor Indicators (FBI): upon capture (chelation) of Ba^{2+}, the color of its fluorescence emission shifts.

In a previous paper, co-authored by Pablo Herrero (PhD student at the DIPC), Celia Rogero (staff scientist at the CFM and DIPC associate) and Juan José Gomez-Cadenas (Ikerbasque professor at the DIPC), the photochemical properties of the FBI molecules were thoroughly characterized. In the present Nature communication, the same group uses a combination of complementary surface science techniques to unambiguously show that Ba^{2+} ions can be trapped (chelated) in vacuum by a monolayer of FBI. Hence, they used X-ray Photoemission Spectroscopy (XPS) to characterize the chemical changes produced in the FBI by capturing barium. The authors found a shift of 0.5 eV in the binding energy of the O 1s core level between the unchelated and chelated states. This is a fingerprint of the chelation of the crown-ether moiety, which is the main agent in capturing the ion. This same effect took place in three different substrates: Au (111), Cu (111) and Indium Tin Oxide (ITO).



Model of the experiment that has been carried out: the neutrinoless double beta decay (0νββ) of ^{136}Xe produces 2 electrons and a $^{136}Ba^{2+}$ dication. This ion is captured by a FBI molecule deposited on a Au (111) surface and causes its structure to change. The structure variation can be seen in the STM images before (green frame) and after chelation (blue frame).

Thanks to the combination of complementary surface science techniques, we offer the demonstration that Ba^{2+} ions can be trapped (chelated) in vacuum by a monolayer of a crown ether based molecules, in particular a fluorescent bicolor indicators (FBI) which is a chemosensors developed within the NEXT collaboration.

Moreover, by Scanning Tunnelling Microscopy and Spectroscopy (STM-STS) the researchers observe that the ion capture produces a torsion of the molecule and changes the electronic structure, in agreement with the theoretical predictions associated with the fluorescence shift. This rearrangement did not take place upon chelation with other ions, such as Na+. STS, that permits to visualize the Lowest Unoccupied Molecular Orbital (LUMO) and the Highest Occupied Molecular Orbital (HOMO), reveals an increment of the HOMO-LUMO gap of 0.56 eV for the Ba^{2+}-chelated molecule with respect to the free molecule, blue shifted in agreement with the fluorescence spectra.

This study demonstrated the capability of FBIs to chelate Ba^{2+} on surfaces in submonolayer regime and in ultra-high vacuum, which are major steps toward the development of a sensor capable of single barium ion detection. Furthermore, the demonstration of chelation of alkali ions by aza-crown ethers could have implications beyond particle physics: they can be used as photo-switching devices, drug carriers and different ion sensors.

DIPC HIGHLIGHT 2022

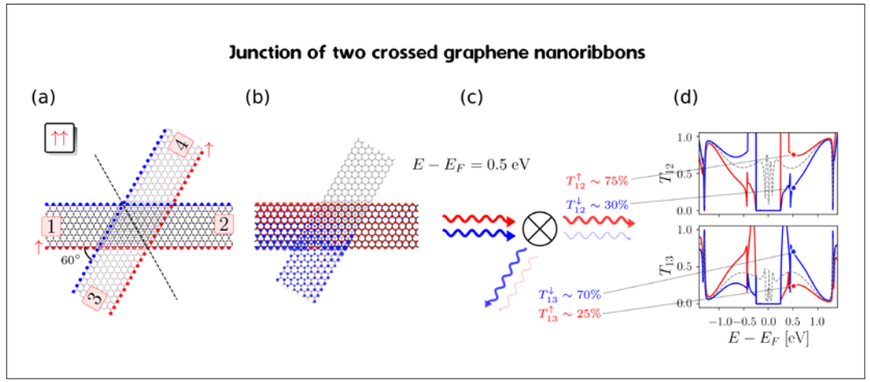
Spin-polarizing electron beam splitter from crossed graphene nanoribbons

Sanz S, Papior N, Giedke G, Sanchez-Portal D, Brandbyge M, and Frederiksen T
Physical Review Letters 129, 037701 (2022)

Graphene has excellent electron mobility, weak spin-orbit coupling, and little nuclear magnetic moment, making it a promising platform for various functionalities, including spin filters, spin qubits, and electron quantum optics. Moreover, thanks to bottom-up fabrication techniques it is possible to synthesize custom-shaped graphene nanostructures. It was shown theoretically not long ago that junctions formed by crossed graphene nanoribbons (GNRs) can act as electron beam splitters. Now Sofía Sanz (along with Géza Giedke and Thomas Frederiksen at DIPC, Daniel Sánchez-Portal at CFM and collaborators in Denmark) shows that the phenomenon not only survives the effect of Coulomb repulsion, but that the magnetism at zigzag edges can lead to substantial spin polarization in the electron transmission.

The idea is summarized in the figure: The junction is formed by two GNRs with zigzag terminations rotated 60 degrees with respect to each other (so that the junction is in the energetically preferable AB stacking configuration of Bernal graphite). The edge states are spin polarized due to a Hubbard-U interaction, which the authors treat self-consistently in mean field. The authors computed spin- and energy-resolved transmission probabilities between any pair of electrodes using Green's functions techniques. The beam-splitting effect survives, with the important caveat that a transport gap opens at low energies due to correlations. More remarkably, the split electron beams may become highly polarized in spin. The effect is generically present even for a range of different twist angles between the ribbons.

The biggest challenge of this proposal is the ability to control the specific spin configuration and device geometry. Nevertheless, as the authors point out, the important point of their study is that the spin configurations are robust enough to be probed by transition current pulses. Although the proposed devices are ahead of current experiments, the authors envision applications of this discovery in spintronics and solid-state-based quantum technologies that are, maybe, not too far from realization.



(a) Transport setup of two crossed ZGNRs overlaid with the self-consistent solution for the up (red) and down (blue) spin-density distributions. Electrodes 1–4 are indicated. (b) Spin-resolved density of states of scattering states incoming from electrode 1 for the solution in a, computed at $E - E_F = 0.5$ eV. The dominant spin on each site at this energy is shown in red for up spins and in blue for down spins. (c) Sketch of incoming and outgoing waves through the scattering center and the corresponding transmission probabilities from calculations. (d) Calculated energy-dependent transmission functions, where the red (blue) curves correspond to the up (down) spin components with on-site interaction U = 3 eV; the unpolarized case (U = 0) is indicated by dashed lines.

Junctions composed of two crossed zigzag graphene nanoribbons (GNRs) are theoretically shown to act as spin-polarizing electron beam splitters: incoming electron waves in one GNR can be split coherently into propagating waves in two outgoing terminals with strongly spin-dependent amplitude and zero back-scattering

DIPC HIGHLIGHT 2022

Macrocyclic polymers: synthesis, purification, properties and applications

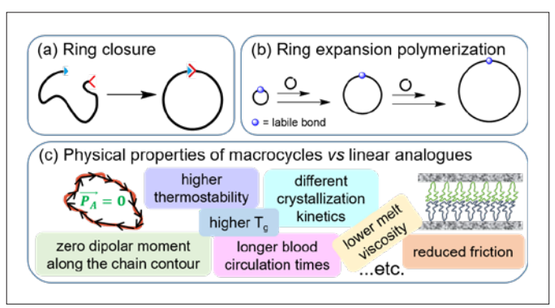
Ochs J, Pagnacco CA, and Barroso-Bujans F
Progress in Polymer Science 134, 101606 (2022)

Cyclic polymers today are at the forefront of macromolecular science. This is because cyclic polymers present intriguing physical and chemical properties given only by the absence of end groups and their circular architecture. The enormous research carried out on synthetic polymers has been important to understand their property-structure relationships.

This has only been possible thanks to innovative advances in organic synthesis and catalysis, creating a variety of pathways to cyclization of preformed chains through ring-closure (RC) strategies and ring-expansion polymerization (REP) of various monomers, as depicted in the figure. RC consists in the closure of a preformed polymer chain by using efficient end-group reactions. It can be unimolecular or bimolecular, and homodifunctional or heterodifunctional. In REP the monomer is incorporated into a preformed cyclic structure that is held together by a relatively labile bond (e.g., organometallic or electrostatic). The cyclic structure is maintained throughout the chain growth. Therefore, this process does not suffer from entropic penalties associated to the reaction between two terminal groups, as it occurs in the RC method.

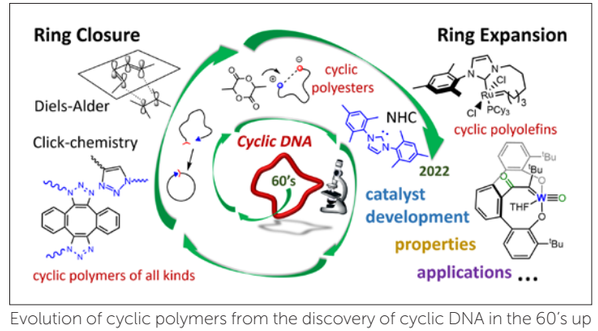
Today, there exists a vast collection of synthetic methods for producing a variety of cyclic polymers. The advent of "click" chemistry and the sophistication of coupling techniques has greatly increased the possibility of ring formation by reaction of a wide variety of functional groups. In particular, metal-free and light-assisted techniques have provided significant advantages in this field. At present, cyclic polymers have found potential utility in the biomedical and pharmacological fields, surface chemistry, as well as plastic and electronic industry. In the long-term, versatile cyclic polymers with useful, autonomous and smart functions are expected to be produced with potential applications in broader scientific fields.

In this extensive review with more than 300 references, scientists from the Donostia International Physics Center (DIPC) and Centro de Física de Materiales (CFM) report recent advances in the synthesis and purification of cyclic (bio)polymers, together with a very comprehensive historical revision of the synthesis methods used to date. Emphasis on modern catalysts is made in REP, whereas the implementation of modern organic reactions appears in RC methods. This review also describes physical and biological properties of cyclic (bio)polymers and recent investigations of their applications in surface science, colloids and polymer networks, including own research developed at DIPC and CFM.



(a) and (b) Synthetic routes to the formation of cyclic polymers. (c) Some examples of their physical properties compared to linear analogues.

The advent of "click" chemistry and the sophistication of coupling techniques has greatly increased the possibility of ring formation



Evolution of cyclic polymers from the discovery of cyclic DNA in the 60's up to date thanks to the development of synthetic routes and powerful catalysts.

Review on cyclic polymers with more than 300 references

DIPC HIGHLIGHT 2022

Engineering quantum states and electronic landscapes through surface molecular nanoarchitectures

Piquero-Zulaica I, Lobo-Checa J, Abd El-Fattah ZM,
Ortega JE, Klappenberger F, Auwarter W, and Barth JV
Reviews of Modern Physics 94, 045008 (2022)

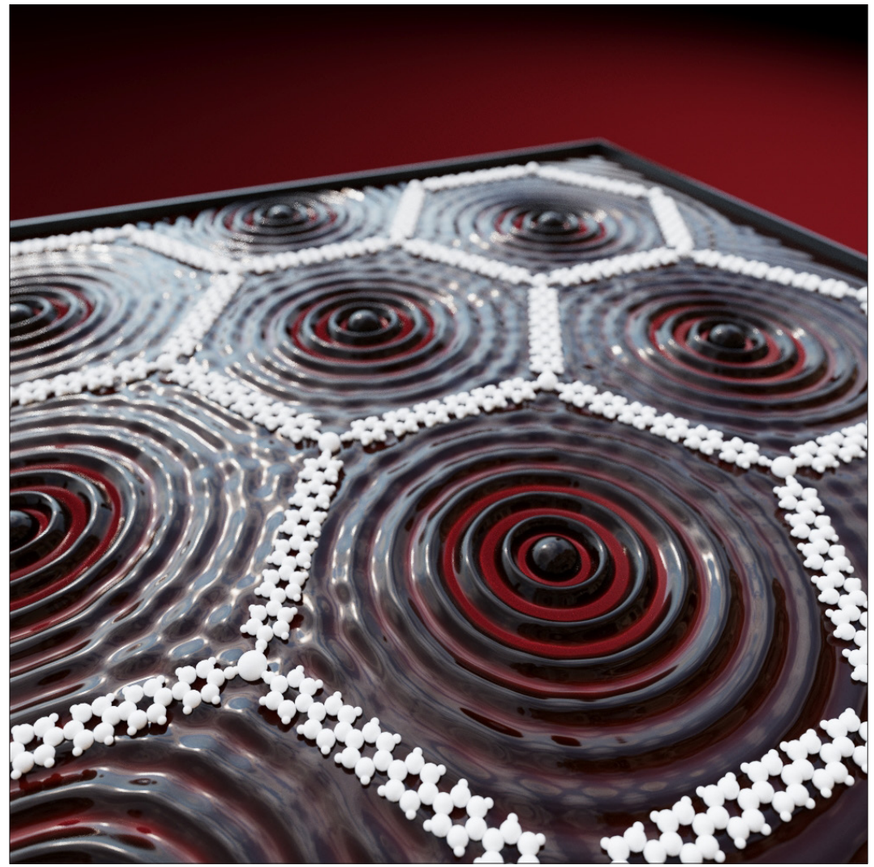
Surfaces are at the frontier of every solid; so they act as support for functional nanostructures and mediate essential physicochemical processes. Actually, they are of utmost relevance because they govern key properties such as the catalytic activity, interfacial charge-transfer, and crystal growth mechanisms. In this quantum and miniaturization era, surfaces and interfaces present distinct electronic states with respect to the bulk, which deserve the scientific community attention as new fundamental properties keep continuously emerging from them.

A fruitful collaboration between scientists in San Sebastián at CFM and DIPC, Zaragoza at INMA and Munich at TUM, led by Dr I. Piquero-Zulaica, presents now a complete review on the control of the surface electron confinement on metallic surfaces. This overview summarizes three decades of global research activity focused on the shaping and tailoring of two-dimensional electron gases (2DEG) by means of patterning with atoms or molecular scaffolds. Such nanostructures and arrays are obtained via self-assembly or atomistic manipulation protocols, promoting the emergence of distinct phenomena in the quantum regime, such as quantum confinement and quasiparticle scattering on different nanopatterned metal surfaces.

Iconic examples in the form of quantum corrals and artificial lattices can induce exotic properties, such as Dirac cones or flat bands, topological edge states or fractal behavior to name a few. The novelty of this work lies in the application of supramolecular chemistry principles to create low-dimensional functional nanostructures to tailor 2DEGs at the interface. These organic nanoarchitectures are more malleable and versatile than atoms, up to the point that new surface band structures emerge. These molecular arrays allow us to investigate relevant physical phenomena, like discretization, quantum coupling, and exotic renormalizations to the energy and effective mass of these bands.

In this work, the team presents these fundamental findings mainly as a combination of scanning probe microscopy and photoemission techniques, which are complemented with theoretical modelling. The full characterization of the electronic properties of these nanoarchitectures and their implications brings within reach the prospect of total control over surface electron confinement and their associated emergent quantum states.

The novelty of this work lies in the application of supramolecular chemistry principles to create low-dimensional functional nanostructures to tailor two-dimensional electron gases (2DEGs) at the interface



Surfaces of solid-state materials can be manipulated to fashion quantum dots and bespoke electronic properties. This review provides an overview of the work to shape two-dimensional electron gasses at the metal surfaces by means of patterning with molecule-based nanostructures formed via supramolecular self-assembly or atomistic manipulation protocols, giving rise to distinct phenomena in the quantum regime.

DIPC HIGHLIGHT 2022

All topological bands of all nonmagnetic stoichiometric materials

Vergniory MG, Wieder BJ, Elcoro L, Parkin SSP, Felser C, Bernevig BA, and Regnault N
Science 376, 816 (2022)

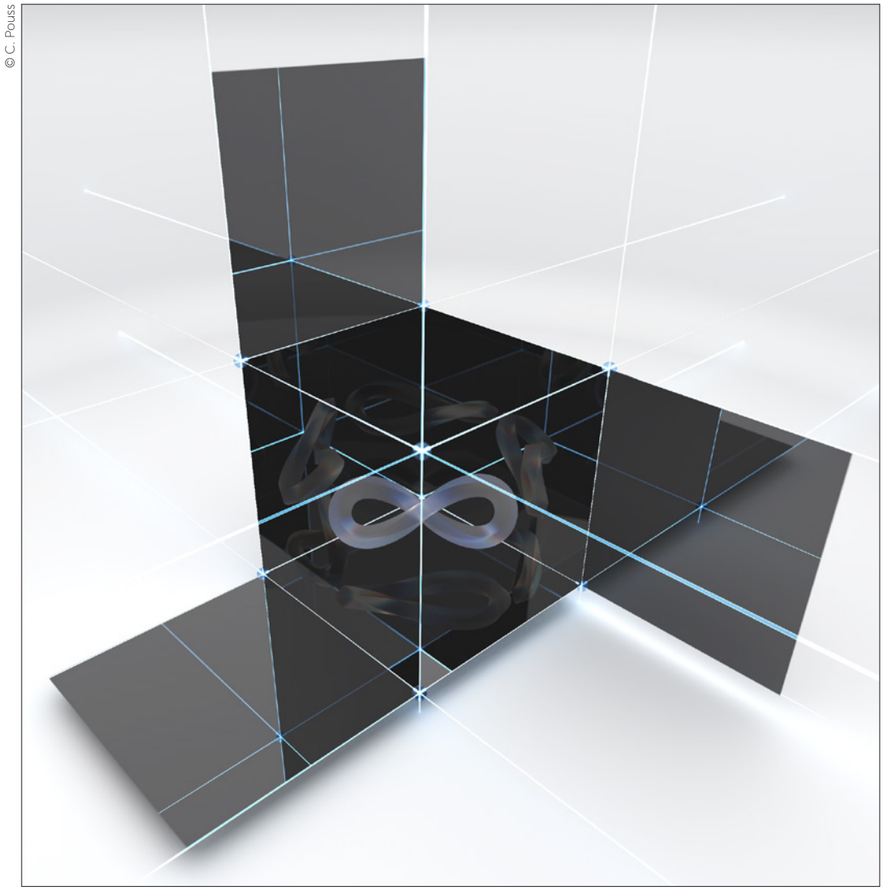
Since the discovery of the quantum Hall effect 40 years ago solid-state physicists have come to realize that there are phases of matter and transitions between them which do not admit descriptions in terms of local order parameters. The last 15 years have witnessed the discovery of many of these topological phases in crystalline solids. Thanks to important technical development in recent years the search of these phases in real materials can be made more systematic, at least from the theory standpoint.

Now Maia Garcia-Vergniory writing *in Science* (in collaboration with researchers in Germany, USA, Spain and France) reports the completion of the topological classification of all known non-magnetic materials following topological quantum chemistry formalism and symmetry-based indicators. The new catalogue is publicly accessible in an upgraded version of the Topological Materials Database (https://topologicalquantumchemistry.com).

The authors performed first-principles calculations in the 96,196 processable entries of the Inorganic Crystal Structure Database; about 75% of them produced converged (non-magnetic) electronic structures after including spin-orbit coupling. The conclusion of the study is that 90% of these electronic structures contain at least one (stable or fragile) topological band, two thirds of bands across all materials exhibit stable topology (of the type of 3D strong/weak topological insulators, topological crystalline insulators, or higher-order topological insulators), and half of the studied compounds are topological at the intrinsic Fermi level. These numbers represent only a lower bound, as there are topological phases which cannot be detected by symmetry-based indicators.

The characterization of band topology away from the Fermi surface is useful for many experimental techniques such as ARPES or more recent pump-probe experiments. The authors indicate that the large number of experimentally accessible materials with stable topological bands away from the Fermi level suggests that many of the surface resonances observed in ARPES are in fact of topological origin; that is the case of Bi_2Mg_3, which the authors discuss in some detail.

The authors highlight many other examples of material candidates in which their investigations have revealed or provided a new context for topological features within experimental reach. One particularly interesting case is the transition-metal chalcogenide Ta_2NiSe_7, which is prone to an incommensurate charge density wave (CDW) instability at low temperatures, and whose normal phase the authors find to be a 3D topological insulator. A natural question then is if the CDW gap is also topological, and in that case, what are the consequences for the new collective modes and the electro-magnetic response of the system (a prime example of the interplay between topology and electronic correlations). If this example is not intriguing enough, the readers of the Science paper are likely to find other examples to their taste.



Mobius strips are visible from all angles of the cube above, representing the ubiquity of topological phases in solid-state materials.

Topology is everywhere

DIPC HIGHLIGHT 2022

Atom scattering as a probe of the surface electron-phonon interaction at conducting surfaces

Manson JR, Benedek G, and Miret-Artes S
Surface Science Reports 77, 100552 (2022)

A surface is made of atoms. And atoms vibrate. But, at any instant of time not all atoms in a solid vibrate at the same frequency and amplitude, nor with the same energy. Over time the vibrational energy of any specific atom will also vary randomly. It follows that at a given temperature there will exist a distribution of energies for the constituent atoms about an average energy. With rising temperature, this average energy increases, and, in fact, the temperature of a solid is really just a measure of the average vibrational activity of atoms.

Many properties and processes in solids are manifestations of this vibrational atomic motion. In most solids the principal mode of energy assimilation is by the increase in vibrational energy of the atoms.

However, atoms are bonded to other atoms in the solid. Rather than being independent of one another, the vibrations of adjacent atoms are coupled by virtue of the atomic bonding. These vibrations are coordinated in such a way that travelling lattice waves are produced. Lattice waves may be thought of as elastic waves or simply sound waves, having short wavelengths and very high frequencies, which propagate through the crystal at the velocity of sound. The vibrational thermal energy for a material consists of a series of these elastic waves, which have a range of distributions and frequencies. The thermal scattering of free electrons during electronic conduction is by these vibrational waves, and these elastic waves also participate in the transport of energy during thermal conduction. The energy quanta of the vibrational waves themselves are termed phonons.

Since very early on it has been generally understood that low energy atoms are repelled from a crystal surface at distances well in front of the positions of the first layer of atomic cores, and that this repulsive force originated from the Pauli exclusion of electrons in the two weakly overlapping electronic densities, that is to say the overlap of the electron cloud of the atom with the weak and decaying electronic density as it extends outward from the crystal surface. As this repulsive force originates when the incoming atomic electron density attempts to embed itself in the rarefied density of surface electrons, it is a logical assumption that the interaction potential should be proportional to the surface electron density in the region of the classical turning point.

Still, because of the small kinetic energies involved, it is generally accepted that the dominant method of energy transfer in atom-surface collisions is through the creation and annihilation of phonons. The fact that incoming atomic projectiles are repelled by the weak electron cloud far outside the surface means that they do not directly sense the positions and vibrations of the target core atoms, but rather sense the target atoms only indirectly through electronic interactions.

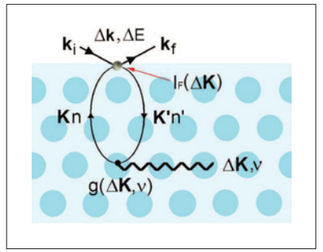


Figure 1. An incident atom in a state of wavevector k_i is inelastically scattered into a final state of wavevector k_F by the overlap vertex $I_F(\Delta K)$ and creates a phonon of wavevector ΔK and branch index ν via a virtual electron-hole pair of states and the electron-phonon vertex term g. (Reprinted with permission from Ref. [46]. Copyright [2016] American Chemical Society).

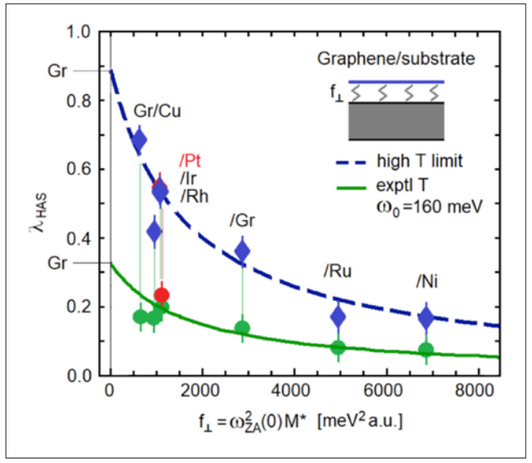


Figure 2. The electron-phonon coupling constant λ_{HAS} plotted as a function of the ZA mode spring constant $f_\perp$ coupling graphene to the substrate. The data are from Ref. [241], with some adjustment; see discussion in the text. The upper dashed-line fitting curve with diamond-shaped data points, as explained in the text, allows the extrapolation of the value $\lambda = 0.89 \pm 0.04$ using the high temperature limit of Eq. (152) for ideally flat free-standing graphene (error bar calculated from the mean-square relative deviation from the fitting curve). Similarly, the lower solid-line curve with circular data points is the result of the Einstein mode approximation of Eq. (161) with ω_0 = 160 meV using the average experimental temperatures and which predicts the value of $\lambda = 0.32 \pm 0.09$ for free standing graphene.

Electron-phonon interaction has great relevance in various nanotechnologies

This strong involvement of the electron density response makes atom scattering significantly different from other commonly used methods, such as electron, X-ray or neutron scattering, all of which directly measure the vibrations of the cores. In atom-surface scattering the atom senses an effective vibrational displacement, that of the surface electrons, and only indirectly the vibrations of the cores.

How to determine the effective vibrational displacement for inelastic atom-surface scattering has been treated in a novel manner using electron-phonon interaction theory. This treatment uses extensions, appropriate for the atom-surface interaction, of the theory of electron-phonon interaction adapted from that used in the theory of superconductivity.

The new work identifies and places into quantitative terms a number of features of the atom-surface interaction potential for both elastic and inelastic scattering. The electron-phonon interaction couples the motion of the electron density to that of the crystal atom cores and allows explicit determination of the effective vibrational displacements sensed by the colliding atomic projectiles. Once the surface vibrational spectrum is known, helium atom scattering permits directly measuring the electron-phonon interaction at surfaces and in general in two-dimensional systems. This answers some fundamental questions such as elucidating the mechanisms of two-dimensional superconductivity. Moreover, electron-phonon interaction has great relevance in various nanotechnologies, and on the nanometric scale what happens at the surface is far more important than what happens in the bulk.

Publications

1 **Omnidirectional spin-to-charge conversion in graphene/$NbSe_2$ van der Waals heterostructures.**
Ingla-Aynes J, Groen I, Herling F, Ontoso N, Safeer CK, de Juan F, Hueso LE, Gobbi M, and Casanova F.
2D Materials 9, 045001 (2022).

2 **Molecular optomechanics approach to surface-enhanced Raman scattering.**
Esteban R, Baumberg JJ, and Aizpurua J.
Accounts of Chemical Research 55, 1889 (2022).

3 **Predicting the second-order nonlinear optical responses of organic materials: the role of dynamics.**
Castet F, Tonnele C, Muccioli L, and Champagne B.
Accounts of Chemical Research 55, 3716 (2022).

4 **Intrinsic ferromagnetism in 2D Fe2H with a high Curie temperature.**
Ding SC, Yan X, Bergara A, Zhang XH, Liu Y, and Yang GC.
ACS Applied Materials & Interfaces 14, 44745 (2022).

5 **Hydrophobic gold nanoparticles with intrinsic chirality for the efficient fabrication of chiral plasmonic nanocomposites.**
Kowalska N, Bandalewicz F, Kowalski J, Gomez-Grana S, Bagiriski M, Pastoriza-Santos I, Grzelczak M, Matraszek J, Perez-Juste J, and Lewandowski W.
ACS Applied Materials & Interfaces 14, 50013 (2022).

6 **Size- and ligand-dependent transport of nanoparticles in matricaria chamomilla as demonstrated by mass spectroscopy and X-ray fluorescence imaging.**
Liu Y, Kornig C, Qi B, Schmutzler O, Staufer T, Sanchez-Cano C, Magel E, White JC, Feliu N, Gruner F, and Parak WJ.
ACS Nano 16, 12941 (2022).

7 Addressing electron spins embedded in metallic graphene nanoribbons.
Friedrich N, Menchon RE, Pozo I, Hieulle J, Vegliante A, Li JC, Sanchez-Portal D, Pena D, Garcia-Lekue A, and Pascual JI.
ACS Nano 16, 14819 (2022).

8 Theory of borazine-derived nanothreads: enumeration, reaction pathways, and piezoelectricity.
Wang T, Crespi VH, Xu ES, Chen B, and Hoffmann R.
ACS Nano 16, 15884 (2022).

9 Role of the magnetic anisotropy in atomic-spin sensing of 1D molecular chains.
Wackerlin C, Cahlik A, Goikoetxea J, Stetsovych O, Medvedeva D, Redondo J, Svec M, Delley B, Ondracek M, Pinar A, et al.
ACS Nano 16, 16402 (2022).

10 Chiral transport of hot carriers in graphene in the quantum hall regime.
Cao B, Grass T, Gazzano O, Ashokbhai Patel K, Hu J, Muller M, Huber-Loyola T, Anzi L, Watanabe K, Taniguchi T, et al.
ACS Nano 16, 18200 (2022).

11 Thickness- and twist-angle-dependent interlayer excitons in metal monochalcogenide heterostructures.
Zheng WK, Xiang L, de Quesada FA, Augustin M, Lu ZG, Wilson M, Sood A, Wu F, Shcherbakov D, Memaran S, and Oliveira TVAGD.
ACS Nano 16, 18695 (2022).

12 Germanium monosulfide as a natural platform for highly anisotropic THz polaritons.
Norenberg T, Alvarez-Perez G, Obst M, Wehmeier L, Hempel F, Klopf JM, Nikitin AY, Kehr SC, Eng LM, Alonso-Gonzalez P, et al.
ACS Nano 16, 20174 (2022).

13 Interlayer coupling of a two-dimensional kondo lattice with a ferromagnetic surface in the antiferromagnet $CeCo_2P_2$.
Poelchen G, Rusinov IP, Schulz S, Guttler M, Mende M, Generalov A, Usachov DY, Danzenbacher S, Hellwig J, Peters M, et al.
ACS Nano 16, 3573 (2022).

14 A chirality-based quantum leap.
Aiello CD, Abendroth JM, Abbas M, Afanasev A, Agarwal S, Banerjee AS, Beratan DN, Belling JN, Berche B, Botana A.
ACS Nano 16, 4989 (2022).

15 The magnetic genome of two-dimensional van der Waals materials.
Wang QH, Bedoya-Pinto A, Blei M, Dismukes AH, Hamo A, Jenkins S, Koperski M, Liu Y, Sun QC, Telford EJ, et al.
ACS Nano 16, 6960 (2022).

16 Neat protein single-chain nanoparticles from partially denatured BSA.
de Molina PM, Le TP, Iturrospe A, Gasser U, Arbe A, Colmenero J, and Pomposo JA.
ACS Omega 7, 42163 (2022).

17 Detecting majorana zero modes via strong field dynamics.
Baldelli N, Bhattacharya U, Gonzalez-Cuadra D, Lewenstein M, and Grass T.
ACS Omega 7, 47424 (2022).

18 Active motion induced by random electromagnetic fields.
Luis-Hita J, Saenz JJ, and Marques MI.
ACS Photonics 9, 1008 (2022).

19 Active tuning of highly anisotropic phonon polaritons in Van der Waals crystal slabs by gated graphene.
Alvarez-Perez G, Gonzalez-Moran A, Capote-Robayna N, Voronin KV, Duan JH, Volkov VS, Alonso-Gonzalez P, and Nikitin AY.
ACS Photonics 9, 383 (2022).

20 Ultrafast plasmonic response ensured by atomic scale confinement.
Tanaka S, Yoshida T, Watanabe K, Matsumoto Y, Yasuike T, Novko D, Petrovic M, and Kralj M.
ACS Photonics 9, 837 (2022).

21 Decoupling of glassy dynamics from viscosity in thin supported Poly(n-butyl methacrylate) films.
Chowdhury M, Monnier X, Cangialosi D, and Priestley RD.
ACS Polymers Au 2, 333 (2022).

22 Strong Rashba effect and different f–d hybridization phenomena at the surface of the heavy-fermion superconductor $CeIrIn_5$.
Mende M, Ali K, Poelchen G, Schulz S, Mandic V, Tarasov AV, Polley C, Generalov A, Fedorov AV, Guttler M, et al.
Advanced Electronic Materials 8, 2100768 (2022).

23 Designing artificial fluorescent proteins: squaraine-LmrR biophosphors for high performance deep-red biohybrid light-emitting diodes.
de Ferrara S, Mejias SH, Liutkus M, Renno G, Stella F, Kociolek I, Fuenzalida-Werner JP, Barolo C, Coto PB, Cortajarena AL, and Costa RD.
Advanced Functional Materials 17, 2111381 (2022).

24 Boosting the stimulated emission properties of host: guest polymer blends by inserting chain twists in the host polymer.
Sun C, Bai LB, Roldao JC, Burgos-Caminal A, Borrell-Grueiro O, Lin JY, Huang W, Gierschner J, Gawelda W, Banares L, and Cabanillas-Gonzalez J.
Advanced Functional Materials 32, 2206723 (2022).

25 Revealing intrinsic superconductivity of the Nb/$BiSbTe_2Se$ interface.
Kudriashov A, Babich I, Hovhannisyan RA, Shishkin AG, Kozlov SN, Fedorov A, Vyalikh DV, Khestanova E, Kupriyanov MY, and Stolyarov VS.
Advanced Functional Materials 32, 2209853 (2022).

26 Active and passive tuning of ultranarrow resonances in polaritonic nanoantennas.
de Duan JH, Alfaro-Mozaz FJ, Taboada-Gutierrez J, Dolado I, Alvarez-Perez G, Titova E, Bylinkin A, Tresguerres-Mata AIF, Martin-Sanchez J, Liu S, et al.
Advanced Materials 34, 2104954, (2022).

27 Nontrivial doping evolution of electronic properties in ising-superconducting alloys.
Wan W, Wickramaratne D, Dreher P, Harsh R, Mazin II, and Ugeda MM.
Advanced Materials 34, 2200492 (2022).

28 Obstructed surface states as the descriptor for predicting catalytic active sites in inorganic crystalline materials.
Li GW, Xu YF, Song ZD, Yang Q, Zhang YD, Liu J, Gupt U, Suss V, Sun Y, Sessi P, et al.
Advanced Materials 34, 2201328 (2022).

29 Large room temperature anomalous transverse thermoelectric effect in kagome antiferromagnet YMn_6Sn_6.
Roychowdhury S, Ochs AM, Guin SN, Samanta K, Noky J, Shekhar C, Vergniory MG, Goldberger JE, and Felser C.
Advanced Materials 34, 2201350 (2022).

30 Machine-learning spectral indicators of topology.
Andrejevic N, Andrejevic J, Bernevig BA, Regnault N, Han F, Fabbris G, Nguyen T, Drucker NC, Rycroft CH, and Li M.
Advanced Materials 34, 2204113 (2022).

31 Observation of superconducting collective modes from competing pairing instabilities in single-layer $NbSe_2$.
Wan W, Dreher P, Munoz-Segovia D, Harsh R, Guo H, Martinez-Galera AJ, Guinea F, de Juan F, and Ugeda MM.
Advanced Materials 34, 2206078 (2022).

32 Robust magnetic order upon ultrafast excitation of an antiferromagnet.
Lee SE, Windsor YW, Fedorov A, Kliemt K, Krellner C, Schussler-Langeheine C, Pontius N, Wolf M, Atxitia U, Vyalikh DV, and Rettig L.
Advanced Materials Interfaces 9, 2201340 (2022).

33 Tuning the optical properties of Au nanoclusters by designed proteins.
Lopez-Martinez E, Gianolio D, Garcia-Orrit S, Vega-Mayoral V, Cabanillas-Gonzalez J, Sanchez-Cano C, and Cortajarena AL.
Advanced Optical Materials 10, 2101332 (2022).

34 Tailoring accidental double bound states in the continuum in all-dielectric metasurfaces.
Abujetas DR, Olmos-Trigo J, and Sanchez-Gil JA.
Advanced Optical Materials 10, 2200301 (2022).

35 Vectorial bulk-boundary correspondence for 3D photonic chern insulators.
devescovi C, Garcia-Diez M, Bradlyn B, Manes JL, Vergniory MG, and Garcia-Etxarri A.
Advanced Optical Materials 10, 2200475 (2022).

36 Magnetic interplay between π-electrons of open-shell porphyrins and d-electrons of their central transition metal ions.
Sun Q, Mateo LM, Robles R, Ruffieux P, Bottari G, Torres T, Fasel R, and Lorente N.
Advanced Science 9, 2105906 (2022).

37 High-quality graphene using boudouard reaction.
Grebenko AK, Krasnikov DV, Bubis AV, Stolyarov VS, Vyalikh DV, Makarova AA, Fedorov A, Aitkulova A, Alekseeva AA, Gilshtein E, et al.
Advanced Science 9, 2200217 (2022).

38 Ru-catalyzed C-H hydroxylation of tyrosine-containing Di- and tripeptides toward the assembly of L-DOPA derivatives.
Andrade-Sampedro P, Matxain JM, and Correa A.
Advanced Synthesis & Catalysis 364, 2072 (2022).

39 Mapping the networked context of Copernicus, Michelangelo, and della Mirandola in wikipedia.
Miccio LA, Gamez-Perez C, Suarez JL, and Schwartz GA.
Advances in Complex Systems 25, 2240010 (2022).

40 Shape-sensitive inelastic scattering from metallic nanoparticles.
Apell SP, Mukhopadhyay G, Antosiewicz TJ, and Aizpurua J.
Advances in Quantum Chemistry 85, 17 (2022).

41 Separation, identification, and confirmation of cyclic and tadpole macromolecules via UPLC-MS/MS.
O'Neill JM, Mao JL, Haque FM, Barroso-Bujans F, Grayson SM, and Wesdemiotis C.
Analyst 147, 2089 (2022).

42 Hydrogen detection limits and instrument sensitivity of high-resolution broadband neutron spectrometers.
Scatigno C, Zanetti M, Rudic S, Senesi R, Andreani C, Gorini G, and Fernandez-Alonso F.
Analytical Chemistry 94, 5023 (2022).

43 Near-unity triplet generation promoted via spiro-conjugation.
Lv M, Lu XC, Jiang YR, Sandoval-Salinas ME, Casanova D, Sun HT, Sun ZR, Xu JH, Yang YJ, and Chen JQ.
Angewandte Chemie-International Edition 61, e202113190 (2022).

44 Hydrogen tunneling in catalytic hydrolysis and alcoholysis of silanes.
Almenara N, Garralda MA, Lopez X, Matxain JM, Freixa Z, and Huertos MA.
Angewandte Chemie-International Edition 61, e202204558 (2022).

45 Reply to the correspondence on "How aromatic are molecular nanorings? The case of a six-porphyrin nanoring".
Casademont-Reig I, Soriano-Agueda L, Ramos-Cordoba E, Torrent-Sucarrat M, and Matito E.
Angewandte Chemie-International Edition 61, e202206836 (2022).

46 The heaviest bottleable metallylone: synthesis of a monatomic, zero-valent lead complex ("plumbylone").
Xu J, Pan S, Yao S, Frenking G, and Driess M.
Angewandte Chemie-international Edition 61, e2022094 (2022).

47 Superconducting proximity effect in d-wave cuprate/graphene heterostructures.
Perconte D, Bercioux D, Dlubak B, Seneor P, Bergeret FS, and Villegas JE.
Annalen Der Physic 534, 2100559 (2022).

48 Assessing cellular uptake of exogenous coenzyme Q(10) into human skin cells by x-ray fluorescence imaging.
Staufer T, Schulze ML, Schmutzler O, Kornig C, Welge V, Burkhardt T, Vietzke JP, Vogelsang A, Weise JM, Blatt T, et al.
Antioxidants 11, 1532 (2022).

49 Temperature-dependent critical spin-orbit field for orthogonal switching in antiferromagnets.
Rama-Eiroa R, Otxoa RM, and Atxitia U.
Applied Physics Letters 121, 132401 (2022).

50 Unraveling the effects of Fe and Mn promoters on the tungstated zirconia catalyst: a DFT study.
Madrigal-Carrillo KG, Rodriguez JI, Hernandez-Pichardo ML, and Jimenez-Izal E.
Applied Surface Science 599, 154052 (2022).

51 The miniJPAS Survey: detection of the double-core Lya morphology for two high-redshift QSOs.
Rahna PT, Zheng ZY, Chies-Santos AL, Cai Z, Spinoso D, Marquez I, Overzier R, Abramo LR, Bonoli S, Kehrig C, et al.
Astronomy & Astrohysics 668, A148 (2022).

52 J-PLUS: spectral evolution of white dwarfs by PDF analysis.
Lopez-Sanjuan C, Tremblay PE, Ederoclite A, Ramio HV, Carrasco JM, Varela J, Cenarro AJ, Marin-Franch A, Civera T, Daflon S, et al.
Astronomy & Astrophysics 658, A79 (2022).

53 J-PLUS: support vector machine applied to STAR-GALAXY-QSO classification.
Wang C, Bai Y, Lopez-Sanjuan C, Yuan H, Wang S, Liu J, Sobral D, Baqui PO, Martin EL, Galarza CA, et al.
Astronomy & Astrophysics 659, A144 (2022).

54 J-PLUS: stellar parameters, C, N, Mg, Ca, and [α/Fe] abundances for two million stars from DR1.
Yang L, Yuan HB, Xiang MS, Duan FQ, Huang Y, Liu JF, Beers TC, Galarza CA, Daflon S, Fernandez-Ontiveros JA, et al.
Astronomy & Astrophysics 659, A181 (2022).

55 Black hole virial masses from single-epoch photometry The miniJPAS test case.
Chaves-Montero J, Bonoli S, Trakhtenbrot B, Fernandez-Centeno A, Queiroz C, Diaz-Garcia LA, Delgado RMG, Hernan-Caballero A, Hernandez-Monteagudo C, Lopen-Sanjuan C, et al.
Astronomy & Astrophysics 660, A95 (2022).

56 The miniJPAS survey: identification and characterization of the emission line galaxies down to z < 0.35 in the AEGIS field.
Martinez-Solaeche G, Delgado RMG, Garcia-Benito R, Diaz-Garcia LA, Rodriguez-Martin JE, Perez E, de Amorim A, Puertas SD, Sodre L, Sobral D, et al.
Astronomy & Astrophysics 661, A99 (2022).

57 Confirmation of a metallicity spread amongst first population stars in globular clusters.
Lardo C, Salaris M, Cassisi S, and Bastian N.
Astronomy & Astrophysics 662, A117 (2022).

58 J-PLUS: support vector regression to measure stellar parameters.
Wang C, Bai Y, Yuan H, Liu J, Fernandez-Ontiveros JA, Coelho PRT, Jimenez-Esteban F, Galarza CA, Angulo RE, Cenarro AJ, et al.
Astronomy & Astrophysics 664, A38 (2022).

59 Godzilla, a monster lurks in the sunburst galaxy.
Diego JM, Pascale M, Kavanagh BJ, Kelly P, Dai L, Frye B, and Broadhurst T.
Astronomy & Astrophysics 665, A134 (2022).

60 The miniJPAS survey: white dwarf science with 56 optical filters.
Lopez-Sanjuan C, Tremblay PE, Ederoclite A, Ramio HV, Cenarro AJ, Marin-Franch A, Varela J, Akras S, Guerrero MA, Jimenez-Esteban FM, et al.
Astronomy & Astrophysics 665, A151 (2022).

61 The miniJPAS survey: a search for extreme emission-line galaxies.
Iglesias-Paramo J, Arroyo A, Kehrig C, Vilchez JM, Puertas SD, Perez-Montero E, Breda I, Jimenez-Teja Y, Lopez San Sanjuan C, Lumbreras-Calle A, et al.
Astronomy & Astrophysics 665, A95 (2022).

62 J-PLUS: discovery and characterisation of ultracool dwarfs using virtual observatory tools II. Second data release and machine learning methodology.
Mas-Buitrago P, Solano E, Gonzalez-Marcos A, Rodrigo C, Martin EL, Caballero JA, Jimenez-Esteban F, Cruz P, Ederoclite A, Ordieres-Mere J, et al.
Astronomy & Astrophysics 666, A147 (2022).

63 The miniJPAS survey galaxy populations in the most massive cluster in miniJPAS: mJPC2470-1771.
Rodriguez-Martin JE, Delgado RMG, Martinez-Solaeche G, Diaz-Garcia LA, de Amorim A, et al.
Astronomy & Astrophysics 666, A160 (2022).

64 The miniJPAS survey the role of group environment in quenching star formation.
Delgado RMG, Rodriguez-Martin JE, Diaz-Garcia LA, de Amorim A, Garcia-Benito R, Martinez-Solaeche G, Lopes PAA, Maturi M, Perez E, Cid Fernandes R, et al.
Astronomy & Astrophysics 666, A84 (2022).

65 J-PLUS: uncovering a large population of extreme [OIII] emitters in the local universe.
Lumbreras-Calle A, Lopez-Sanjuan C, Sobral D, Fernandez-Ontiveros JA, Vilchez JM, Hernan-Caballero A, Akhlaghi M, Diaz-Garcia LA, Alcaniz J, Angulo RE, et al.
Astronomy & Astrophysics 668, A60 (2022).

66 TOPz: photometric redshifts for J-PAS.
Laur J, Tempel E, Tamm A, Kipper R, Liivamagi LJ, Hernan-Caballero A, Muru MM, Chaves-Montero J, Diaz-Garcia LA, Turner S, et al.
Astronomy & Astrophysics 668, A8 (2022).

67 Suppressing variance in 21 cm signal simulations during reionization.
Giri SK, Schneider A, Maion F, and Angulo RE.
Astronomy & Astrophysics 669, A6 (2022).

68 An analytic model for the subgalactic matter power spectrum in fuzzy dark matter halos.
de Kawai H, Oguri M, Amruth A, Broadhurst T, and Lim J.
Astrophysical Journal 925, 61 (2022).

69 The magnetic field environment of active region 12673 that produced the energetic particle events of september 2017.
Yardley SL, Green LM, James AW, Stansby D, and Mihailescu T.
Astrophysical Journal 937, 57 (2022).

70 Expanding the time domain of multiple populations: evidence of nitrogen variations in the similar to 1.5 gyr old star cluster NGC 1783.
de Cadelano M, Dalessandro E, Salaris M, Bastian N, Mucciarelli A, Saracino S, Martocchia S, and Cabrera-Ziri I.
Astrophysical Journal Letters 924, L2 (2022).

71 Panic! at the disks: first rest-frame optical observations of galaxy structure at z > 3 with JWST in the SMACS 0723 field.
Ferreira L, Adams N, Conselice CJ, Sazonova E, Austin D, Caruana J, Ferrari F, Verma A, Trussler J, Broadhurst T, et al.
Astrophysical Journal Letters 938, L2 (2022).

72 Unscrambling the lensed galaxies in JWST images behind SMACS 0723.
Pascale M, Frye BL, Diego J, Furtak LJ, Zitrin A, Broadhurst T, Conselice CJ, Dai L, Ferreira L, Adams NJ, et al.
Astrophysical Journal Letters 938, L6 (2022).

73 JWST imaging of Earendel, the extremely magnified star at redshift z=6.2.
Welch B, Coe D, Zackrisson E, de Mink SE, Ravindranath S, Anderson J, Brammer G, Bradley L, Yoon J, Kelly P, et al.
Astrophysical Journal Letters 940, L1 (2022).

74 Early results from GLASS-JWST. VIII. An extremely magnified blue supergiant star at redshift 2.65 in the A2744 cluster field.
Chen WL, Kelly PL, Treu T, Wang X, Roberts-Borsani G, Keen A, Windhorst RA, Zhou R, Bradac M, Brammer G, et al.
Astrophysical Journal Letters 940, L54 (2022).

75 Spin polarization of electrons in two-color XUV + optical photoionization of atoms.
Kabachnik NM, and Sazhina IP.
Atoms 10, 66 (2022).

76 Cognitive functions are not reducible to biological ones: the case of minimal visual perception.
Arnellos A, and Moreno A.
Biology and Philosophy 37, 35 (2022).

77 Brain virtual histology with X-ray phase-contrast tomography part II: 3D morphologies of amyloid-β plaques in Alzheimer's disease models.
Chourrout M, Roux M, Boisvert C, Gislard C, Legland D, Arganda-Carreras I, Olivier C, Peyrin F, Boutin H, Rama N, et al.
Biomedical Optics Express 13, 1640 (2022).

78 Phase separation in amino acid mixtures is governed by composition.
de Sancho D.
Biophysical Journal 121, 4119 (2022).

79 Real-time monitoring of breath biomarkers with a magnetoelastic contactless gas sensor: a proof of concept.
Pena A, Aguilera JD, Matatagui D, de la Presa P, Horrillo C, Hernando A, and Marin P.
Biosensors-Basel 12, 871 (2022).

80 An increase in spontaneous activity mediates visual habituation.
Mille JEK, Miller BR, O'Neil DA, and Yuste R.
Cell Reports 39, 110751 (2022).

81 Not dark yet for strong light-matter coupling to accelerate singlet fission dynamics.
Climent C, Casanova D, Feist J, and Garcia-Vidal FJ.
Cell Reports Physical Science 3, 100841 (2022).

82 A quantitative biophysical principle to explain the 3D cellular connectivity in curved epithelia.
Gomez-Galvez P, Vicente-Munuera P, Anbari S, Tagua A, Gordillo-Vazquez C, Andres-San Roman JA, Franco-Barranco D, Palacios AM, Velasco A, Capitan-Agudo C, et al.
Cell Systems 13, 631 (2022).

83 A patchy particle model for C-S-H formation.
Prabhu A, Dolado JS, Koenders EAB, Zarzuela R, Mosquera MJ, Garcia-Lodeiro I, and Blanco-Varela MT.
Cement and Concrete Research 152, 106658 (2022).

84 Coexistence of antiferro- and ferrimagnetism in the spinel $ZnFe_2O_4$ with an inversion degree δ lower than 0.3.
Cobos MA, de la Presa P, Puente-Orench I, Llorente I, Morales I, Garcia-Escorial A, Hernando A, and Jimenez JA.
Ceramics International 48, 12048 (2022).

85 Triple bonding between beryllium and nitrogen in HNBeCO.
Wang LN, Pan S, Wang GJ, Zeng XQ, Zhou MF, and Frenking G.
Chemical Communications 58, 8532 (2022).

86 Bio-inspired membranes for adsorption of arsenic via immobilized L-cysteine in highly hydrophilic electrospun nanofibers.
Picon D, Torasso N, Baudrit JRV, Cerveny S, and Goyanes S.
Chemical Engineering Research & Design 185, 108 (2022).

87 O_2 on Ag(110): A puzzle for exchange-correlation functionals.
Loncarica I, Alducin M, and Juaristi JI.
Chemical Physics 554, 111424 (2022).

88 Cluster approach to scattering in MoS_2 photoemission.
Ambrosio MJ, Plesiat E, Decleva P, Echenique PM, Muino RD, and Martin F.
Chemical Physics 557, 111476 (2022).

89 Absence of isotope effects in the photo-induced desorption of CO from saturated Pd(111) at high laser fluence.
Muzas AS, Jimenez AS, Ovcar J, Loncaric I, Alducin M, and Juaristi JI.
Chemical Physics 558, 111518 (2022).

90 Light-driven reduction of aromatic olefins in aqueous media catalysed by aminopyridine cobalt complexes.
Casadevall C, Pascual D, Aragon J, Call A, Casitas A, Casademont-Reig I, and Lloret-Fillol J.
Chemical Science 13, 4270 (2022).

91 Unparalleled selectivity and electronic structure of heterometallic [LnLn'Ln] molecules as 3-qubit quantum gates.
Maniaki D, Garay-Ruiz D, Barrios LA, Martins DOTA, Aguila D, Tuna F, Reta D, Roubeau O, Bo C, and Aromi G.
Chemical Science 13, 5574 (2022).

92 Metal substrate catalysis in the confined space for platinum drug delivery.
Velasco-Lozano S, Alonso-de Castro S, Sanchez-Cano C, Benitez-Mateos AI, Lopez-Gallego F, and Salassa L.
Chemical Science 13, 59 (2022).

93 Conceptual density functional theory under pressure: Part I. XP-PCM method applied to atoms.
Eeckhoudt J, Bettens T, Geerlings P, Cammi R, Chen B, Alonso M, and de Proft F.
Chemical Science 13, 9329 (2022).

94 Enhancing dual-state emission in maleimide fluorophores through fluorocarbon functionalisation.
Pervez M, Pearce AK, Dr. Husband JT, Male L, Torrent-Sucarrat M, and O'Reilly RK.
Chemistry A European Journal 28, e202201877 (2022).

95 High-pressure reaction profiles and activation volumes of 1,3-cyclohexadiene dimerizations computed by the extreme pressure-polarizable continuum model (XP-PCM).
Chen B, Houk KN, and Cammi R.
Chemistry-A European Journal 28, e202200246 (2022).

96 Theory of exciton dynamics in thermally activated delayed fluorescence.
Carreras A, and Casanova D.
ChemPhotoChem 6, e202200066 (2022).

97 Proton and lithium cations linked to π-electron and sigma-electron systems: are such interactions beyond or within the definition of hydrogen/lithium bond?
Samira G, Mohammad A, and Grabowski Slawomir J.
Chemphyschem 223, e202200273 (2022).

98 Experiment and theory clarify: Sc^+ receives one oxygen atom from SO_2 to form ScO^+, which proves to be a catalyst for the hidden oxygen-exchange with SO_2.
de Mercero, JM, Rezabal E, Ugalde JM, Weiske T, and Li JL.
Chemphyschem 23, e202100773 (2022).

99 Diastereoselectivity on intramolecular alder-ene reaction of 1,6-dienes.
de Cozar A.
Chemphyschem 23, e202200377 (2022).

100 Kibble-Zurek mechanism for nonequilibrium phase transitions in driven systems with quenched disorder.
Reichhardt CJO, del Campo A, and Reichhardt C.
Communications Physics 5, 173 (2022).

101 Ultimate speed limits to the growth of operator complexity.
Hornedal N, Carabba N, Matsoukas-Roubeas AS, del Campo A.
Communications Physics 5, 207 (2022).

102 Impact of charge-resonance excitations on CT-mediated J-type aggregation in singlet and triplet exciton states of perylene di-Imide aggregates: A TDDFT Investigation.
Dai YS, Zubiria-Ulacia M, Casanova D, and Negri F.
Computation 10, 18 (2022).

103 First principles calculations of the inorganic halide perovskite $RbSnBr_3$: Optical and thermoelectric properties of its three phases.
Bouchikhi S, Benyahia K, Mehyaoui R, and Touia A.
Computational Condensed Matter 33, e00761 (2022).

104 IrRep: symmetry eigenvalues and irreducible representations of ab initio band structures.
Iraola M, Manes JL, Bradlyn B, Horton MK, Neupert T, Vergniory MG, and Tsirkin SS.
Computer Physics Communications 272, 108226 (2022).

105 π-hole tetrel bonds-lewis acid properties of metallylenes.
Grabowski SJ.
Crystals 12, 112 (2022).

106 Ni(i)-TPA stabilization by hydrogen bond formation on the second coordination sphere: a DFT characterization.
Posada-Perez S, Escayola S, Poater J, Sola M, and Poater A.
Dalton Transactions 51, 12585 (2022).

107 Slow magnetic relaxation in Fe(II) m-terphenyl complexes.
Valentine AJ, Geer AM, Blundell TJ, Tovey W, Cliffe MJ, Davies ES, Argent SP, Lewis W, McMaster J, Taylor LJ, et al.
Dalton Transactions 51, 18118 (2022).

108 Study of the DNA binding mechanism and in vitro activity against cancer cells of iron(III) and aluminium(III) kojic acid derivative complexes.
Lachowicz JI, Mateddu A, Coni P, Caltagirone C, Murgia S, Gibson D, Dalla Torre G, Lopez X, Meloni F, and Pichiri G.
Dalton Transactions 51, 6254 (2022).

109 Optoelectronic properties of a self-assembling rigidly-linked BF_2-curcuminoid bichromophore.
Tonnele C, Catherin M, Giorgi M, Canard G, Casanova D, Castet F, Zaborova E, and Fages F.
Dyes and Pigments 207, 110677 (2022).

110 Identification and measurement of tropical tuna species in purse seiner catches using computer vision and deep learning.
Lekunberri X, Ruiz J, Quincoces I, Dornaika F, Arganda-Carreras I, and Fernandes JA.
Ecological Informatics 67, 101495 (2022).

111 Comments on "What is the radiation before 5G? A correlation study between measurements in situ and in real time and epidemiological indicators in Vallecas, Madrid".
Najera A, Ramis R, Andes FLH, Garcia-Pardo C, Alonso JI, Gonzalez-Rubio J, Hernando A, Martinez JL, and Marcos FV.
Environmental Research 212, 113314 (2022).

112 Unconventional and sustainable synthesis of polymethine dyes: critical overview and perspectives within the framework of the twelve principles of green chemistry.
Antenucci A, Nejrotti S, Plata MJM, Mariotti N, and Barbero N.
European Journal of Organic Chemistry 2022, e202200943 (2022).

113 Reactivity of $B(C_6F_5)_3$ towards glycidol: the formation of branched cyclic polyglycidol structures.
Al Assiri MA, Urreizti EG, Pagnacco CA, de San Roman EG, and Barroso-Bujans F.
European Polymer Journal 171, 111194 (2022).

114 Can aluminum, a non-redox metal, alter the thermodynamics of key biological redox processes? The DPPH-QH(2) radical scavenging reaction as a test case.
Lanuza J, Postils V, and Lopez X.
Free Radical Biology and Medicine 179, 200 (2022).

115 Application of historic datasets to understanding open solar flux and the 20th-century grand solar maximum. 2. Solar observations.
Lockwood M, Owens MJ, Yardley SL, Virtanen IOI, Yeates AR, and Munoz-Jaramillo A.
Frontiers in Astronomy and Space Sciences 9, 976444 (2022).

116 Statistical atlases and automatic labeling strategies to accelerate the analysis of social insect brain evolution.
Arganda S, Arganda-Carreras I, Gordon DG, Hoadley AP, Perez-Escudero A, Giurfa M, and Traniello JFA.
Frontiers in Ecology and Evolution 9, 745707 (2022).

117 Combined DFT and MD simulation protocol to characterize self-healing properties in disulfide-containing materials: polyurethanes and polymethacrylates as casesstudies.
Irigoyen M, Matxain JM, and Ruiperez F.
Frontiers in Materials 9, 859482 (2022).

118 Synthesis of novel hyaluronic acid sulfonated hydrogels using safe reactants: a chemical and biological characterization.
Sturabotti E, Consalvi S, Tucciarone L, Macri E, Di Lisio V, Francolini I, Minichiello C, Piozzi A, Vuotto C, and Martinelli A.
Gels 8, 480 (2022).

119 Studies of the temperature dependence of the structure and magnetism of a hexagonal-bipyramidal dysprosium(III) single-molecule magnet.
Ding YS, Blackmore WJA, Zhai YQ, Giansiracusa MJ, Reta D, Vitorica-Yrezabal I, Winpenny REP, Chilton NF, and Zheng YZ.
Inorganic Chemistry 61, 227 (2022).

120 Enhancing effects of the Cyano group on the C-X···N hydrogen or halogen bond in complexes of X-cyanomethanes with trimethyl amine: $CH_{3-n}(CN)_nX\cdots NMe_3$, (n=0-3; X = H, Cl, Br, I).
Parra RD, and Grabowski SJ.
International Journal of Molecular Sciences 23, 11289 (2022).

121 Total electron detachment and induced cationic fragmentation cross sections for superoxide anion (O_2^-) collisions with benzene (C_6H_6) molecules.
Guerra C, Kumar S, Aguilar-Galindo F, Diaz-Tendero S, Lozano AI, Mendes M, Oller JC, Limao-Vieira P, and Garcia G.
International Journal of Molecular Sciences 23, 1266 (2022).

122 Resolving the mechanism of acoustic plasmon instability in graphene doped by alkali metals.
Marusic L, Kalinic A, Radovic I, Jakovac J, Miskovic ZL, and Despoja V.
International Journal of Molecular Sciences 23, 4770 (2022).

123 Thymosin β4 Is an endogenous iron chelator and molecular switcher of ferroptosis.
Lachowicz JI, Pichiri G, Piludu M, Fais S, Orru G, Congiu T, Piras M, Faa G, Fanni D, Dalla Torre G, et al.
International Journal of Molecular Sciences 23, 551 (2022).

124 Prediction of strong transversal s(TE) exciton-polaritons in C-60 thin crystalline films.
Despoja V, and Marusic L.
International Journal of Molecular Sciences 23, 6943 (2022).

125 Algebraic Lq-norms and complexity-like properties of Jacobi polynomials: degree and parameter asymptotics.
Sobrino N, and Dehesa JS.
International Journal of Quantum Chemistry 122, e26858 (2022).

126 Cementitious materials as promising radiative coolers for solar cells.
Cagnoni M, Tibaldi A, Dolado JS, and Cappelluti F.
Iscience 25, 105320 (2022).

127 Dehydroxylation processing and lasing properties of a Nd alumino-phosphate glass.
de Munoz-Quinonero M, Azkargorta J, Iparraguirre I, Jimenez-Rioboo RJ, Tricot G, Shao CY, Munoz F, Fernandez J, and Balda R.
Journal of Alloys and Compounds 896, 163040 (2022).

128 Zinc glycolate $Zn(OCH_2CH_2O)$: synthesis and structure, spectral and optical properties, electronic structure and chemical bonding.
Krasil'nikov VN, Tyutyunnik AP, Zhukov VP, Baklanova IV, Gyrdasova OI, and Chulkov EV.
Journal of Alloys and Compounds 924, 166320 (2022).

129 Active site dynamics and catalytic mechanism in arabinan hydrolysis catalyzed by GH43 endo-arabinanase from QM/MM molecular dynamics simulation and potential energy surface.
Meelua W, Wanjai T, Thinkumrob N, Olah J, Mujika JI, Ketudat-Cairns JR, Hannongbua S, and Jitonnom J.
Journal of Biomolecular Structure & Dynamics 40, 7439 (2022).

130 AMBER drug discovery boost tools: automated workflow for production free-energy simulation setup and analysis (ProFESSA).
Ganguly A, Tsai H, Fernandez-Pendas M, Lee T, Giese TJ, and York DM.
Journal of Chemical Information and Modeling 62, 6069 (2022).

131 Challenges on optical printing of colloidal nanoparticles.
de Violi IL, Martinez LP, Barella M, Zaza C, Chvatal L, Zemanek P, Gutierrez MV, Paredes MY, Scarpettini AF, Olmos-Trigo J, et al.
Journal of Chemical Physics 156, 034201 (2022).

132 Simple evaluation of dynamic disorder effects on exciton transport.
Carreras A, and Casanova D.
Journal of Chemical Physics 156, 044112 (2022).

133 Does the composition in PtGe clusters play any role in fighting CO poisoning?
Ugartemendia A, Mercero JM, de Cozar A, and Jimenez-Izal E.
Journal of Chemical Physics 156, 174301 (2022).

134 Natural range separation of the Coulomb hole.
Via-Nadal M, Rodriguez-Mayorga M, Ramos-Cordoba E, and Matito E.
Journal of Chemical Physics 156, 184106 (2022).

135 Superconducting $Li_{10}Se$ electride under pressure.
Zhang XH, Zhao YP, Bergara A, and Yang GC.
Journal of Chemical Physics 156, 194112 (2022).

136 Adiabatic electronic flux in molecules and in condensed matter.
Resta R.
Journal of Chemical Physics 156, 204118 (2022).

137 Benchmarking GNOF against FCI in challenging systems in one, two, and three dimensions.
Mitxelena I, and Piris M.
Journal of Chemical Physics 156, 214102 (2022).

138 The contribution of intermolecular spin interactions to the London dispersion forces between chiral molecules.
Geyer M, Gutierrez R, Mujica V, Silva JFR, Dianat A, and Cuniberti G.
Journal of Chemical Physics 156, 234106 (2022).

139 The nature of the polar covalent bond.
Zhao LL, Pan SD, and Frenking G.
Journal of Chemical Physics 157, 034105 (2022).

140 Studying and exploring potential energy surfaces of compressed molecules: a fresh theory from the extreme pressure polarizable continuum model.
Cammi R, and Chen B.
Journal of Chemical Physics 157, 114101 (2022).

141 The Wigner localization of interacting electrons in a one-dimensional harmonic potential.
Telleria-Allika X, Azor ME, Francois G, Bendazzoli GL, Matxain JM, Lopez X, Evangelisti S, and Berger JA.
Journal of Chemical Physics 157, 174107 (2022).

142 Choosing bad versus worse: predictions of two-photon-absorption strengths based on popular density functional approximations.
Choluj M, Alam MM, Beerepoot MTP, Sitkiewicz SP, Matito E, Ruud K, and Zalesny R.
Journal of Chemical Theory and Computation 18, 1046 (2022).

143 Statistical thermodynamics in reversible clustering of gold nanoparticles. A first step towards nanocluster heat engines.
Mezzasalma SA, Kruse J, Ibarra AI, Arbe A, and Grzelczak M.
Journal of Colloid and Interface Science 628, 205 (2022).

144 A study of the performance of classical minimizers in the quantum approximate optimization algorithm.
Fernandez-Pendas M, Combarro EF, Vallecorsa S, Ranilla J, and Rua IF.
Journal of Computational and Applied Mathematics 404, 113388 (2022).

145 The second derivative of the electronic energy with respect to the compression scaling factor in the XP-PCM model: theory and applications to compression response functions of atoms.
Cammi R, and Chen B.
Journal of Computational Chemistry 43, 1176 (2022).

146 Statistics of biased tracers in variance-suppressed simulations.
Maion F, Angulo RE, and Zennaro M.
Journal of Cosmology and Astroparticle Physics 10, 036 (2022).

147 DEMNUni: comparing nonlinear power spectra prescriptions in the presence of massive neutrinos and dynamical dark energy.
Parimbelli G, Carbone C, Bose B, Calabrese M, Carella E, and Zennaro M.
Journal of Cosmology and Astroparticle Physics 11, 041 (2022).

148 Precursor synthesis and properties of iron and lithium co-doped cadmium oxide.
Krasil'nikov V, Zhukov V, Chulkov E, Tyutyunnik A, Dyachkova T, Baklanova I, Gyrdasova O, Zhuravlev N, Chistyakov V, Gao T, et al.
Journal of Electroceramics 48, 127 (2022).

149 Reassessment of thermochemical energy storage in perovskite-like manganites at comparative studies of RP $SrCa_3Mn_3O_{10-d}$ vs. orthorhombic $Sr_{0.25}Ca_{0.75}MnO_{3-d}$.
Antipinskaya EA, Politov BV, Petrova SA, Zhukov VP, Chulkov EV, Suntsov AY, and Kozhevnikov VL.
Journal of Energy Storage 53, 105175 (2022).

150 Bounds on new physics with data of the Dresden-II reactor experiment and COHERENT.
Coloma P, Esteban I, Gonzalez-Garcia MC, Larizgoitia L, Monrabal F, and Palomares-Ruiz S.
Journal of High Energy Physics 5, 037 (2022).

151 Status and perspectives of the PETALO project.
Ferrario P.
Journal of Instrumentation 17, C01057 (2022).

152 Monte Carlo characterization of PETALO, a full-body liquid xenon-based PET detector.
Renner J, Romo-Luque C, Aliaga RJ, Alvarez V, Ballester F, Benlloch-Rodriguez JM, Carrion JV, Cubero D, Diaz J, Esteve R, et al.
Journal of Instrumentation 17, P05044 (2022).

153 Neutron tagging following atmospheric neutrino events in a water Cherenkov detector.
Abe K, Haga Y, Hayato Y, Hiraide K, Ieki K, Ikeda M, Imaizumi S, Iyogi K, Kameda J, Kanemura Y, et al.
Journal of Instrumentation 17, P10029 (2022).

154 Strong coupling effects in a plexciton system of gold nanostars and J-aggregates.
Melnikau D, Samokhvalov P, Sanchez-Iglesias A, Grzelczak M, Nabiev I, and Rakovich YP.
Journal of Luminescence 242, 118557 (2022).

155 Inertial domain wall characterization in layered multisublattice antiferromagnets.
Rama-Eiroa R, Roy PE, Gonzalez JM, Guslienko KY, Wunderlich J, and Otxoa RM.
Journal of Magnetism and Magnetic Materials 560, 169566 (2022).

156 Halogen-free photosensitizers based on meso-enamine-BODIPYs for bioimaging and photodynamic therapy.
Prieto-Montero R, Andres AD, Prieto-Castaneda A, Tabero A, Longarte A, Agarrabeitia AR, Villanueva A, Ortiz MJ, Montero R, Casanova D, and Martinez-Martinez V.
Journal of Materials Chemistry B 11, 169 (2022).

157 Rationalization and tuning of doublet emission in organic radicals.
Tonnele C, and Casanova D.
Journal of Materials Chemistry C 10, 13826 (2022).

158 Highlighting the processing versatility of a silicon phthalocyanine derivative for organic thin-film transistors.
Cranston RR, King B, Dindault C, Grant TM, Rice NA, Tonnele C, Muccioli L, Castet F, Swaraj S, and Lessard BH.
Journal of Materials Chemistry C 10, 485 (2022).

159 Evolutionary kinetic Monte Carlo simulation of anisotropic wet etching of sapphire at different concentrations and temperatures.
Wu GR, Gosalvez MA, and Xing Y.
Journal of Microelectromechanical Systems 31, 249 (2022).

160 Influence of ice formation on the dynamic and thermodynamic properties of aqueous solutions.
Melillo JH, Swenson J, and Cerveny S.
Journal of Molecular Liquids 356, 119039 (2022).

161 $KLaF_4:Nd^{3+}$ doped transparent glass-ceramics processed by spark plasma sintering.
Babu S, Balda R, Fernandez J, Sedano M, Gorni G, Cabral AA, Galusek D, Duran A, and Pascual MJ.
Journal of Non-Crystalline Solids 578, 121289 (2022).

162 Synthesis of bicyclic hemiacetals catalyzed by unnatural densely substituted gamma-dipeptides.
Agirre M, Bello T, Zhou JX, Retamosa MD, and Cossio FP.
Journal of Organic Chemistry 87, 14819 (2022).

163 Influence of the nonprotein amino acid mimosine in peptide conformational propensities from novel amber force field parameters.
Urriolabeitia A, de Sancho D, and Lopez X.
Journal of Physical Chemistry B 126, 2959 (2022).

164 Statistical analysis of photoluminescence decay kinetics in quantum dot ensembles: effects of inorganic shell composition and environment.
Martins JR, Krivenkov V, Bernardo CR, Samokhvalov P, Nabiev I, Yury P, Rakovich YP, and Vasilevskiy MI.
Journal of Physical Chemistry C 126, 20480 (2022).

165 Optical properties of colloidal silver nanowires.
Hamans RF, Parente M, Garcia-Etxarri A, and Baldi A.
Journal of Physical Chemistry C 126, 8703 (2022).

166 Cross determination of exciton coherence length in J-aggregates.
Jumbo-Nogales A, Krivenkov V, Rusakov K, Urban AS, Grzelczak M, and Rakovich YP.
Journal of Physical Chemistry Letters 13, 10198 (2022).

167 Metal-polymer heterojunction in colloidal-phase plasmonic catalysis.
Rogolino A, Claes N, Cizaurre J, Marauri A, Jumbo-Nogales A, Lawera Z, Kruse J, Sanroman-Iglesias M, Zarketa I, Calvo U, at al.
Journal of Physical Chemistry Letters 13, 2264 (2022).

168 Light-driven topological and magnetic phase transitions in thin layer antiferromagnets.
Rodriguez-Vega M, Lin ZX, Leonardo A, Ernst A, Vergniory MG, and Fiete GA.
Journal of Physical Chemistry Letters 13, 4152 (2022).

169 Parallel versus twisted pentacenes: conformational impact on singlet fission.
Papadopoulos I, Reddy SR, Coto PB, Lehnherr D, Thiel D, Thoss M, Tykwinski RR, and Guldi DM.
Journal of Physical Chemistry Letters 13, 5094 (2022).

170 Electron-volt fluctuation of defect levels in metal halide perovskites on a 100 ps time scale.
Wang BP, Chu WB, Wu YF, Casanova D, Saidi WA, and Prezhdo OV.
Journal of Physical Chemistry Letters 13, 5946 (2022).

171 How reliable are modern density functional approximations to simulate vibrational spectroscopies?
Sitkiewicz SP, Zalesny R, Ramos-Cordoba E, Luis JM, and Matito E.
Journal of Physical Chemistry Letters 13, 5963 (2022).

172 Identification and manipulation of defects in black phosphorus.
Harsh R, Mondal S, Sharma D, Bouatou M, Chacon C, Ilyn M, Rogero C, Repain V, Bellec A, Girard Y, et al.
Journal of Physical Chemistry Letters 13, 6276 (2022).

173 Estimating the orientation of 4f magnetic moments by classical photoemission.
Usachov DY, Glazkova D, Tarasov AV, Schulz S, Poelchen G, Bokai KA, Vilkov OY, Dudin P, Kummer K, Kliemt K, et al.
Journal of Physical Chemistry Letters 13, 7861 (2022).

174 Unraveling the ordered phase of the quintessential hybrid perovskite $MAPbI_3$—thermophysics to the rescue.
Marin-Villa P, Arauzo A, Druzbicki K, and Fernandez-Alonso F.
Journal of Physical Chemistry Letters 13, 8422, (2022).

175 Why ultrafast photoinduced CO desorption dominates over oxidation on Ru(0001).
Tetenoire A, Ehlert C, Juaristi JI, Saalfrank P, and Alducin M.
Journal of Physical Chemistry Letters 13, 8516 (2022).

176 The single-point Berry phase in condensed-matter physics.
Resta R.
Journal of Physics A: Mathematical and Theoretical 55, 491001 (2022).

177 Superconducting hydrides on a quantum landscape.
Errea I.
Journal of Physics Condensed Matter 34, 231501 (2022).

178 Energy density as a probe of band representations in photonic crystals.
de Paz MB, Herrera MAJ, Huidobro PA, Alaeian H, Vergniory MG, Bradlyn B, Giedke G, Garcia-Etxarri A, and Bercioux D.
Journal of Physics Condensed Matter 34, 314002 (2022).

179 Carbon-based nanostructures as a versatile platform for tunable π-magnetism.
de Oteyza DG, and Frederiksen T.
Journal of Physics Condensed Matter 34, 443001 (2022).

180 Spin excitations of individual magnetic dopants in an ionic thin film.
Li Z, Delgado F, Du M, He C, Schouteden K, Van Haesendonck C, Janssens E, Arnau A, Lievens P, and Cerda JI.
Journal of Physics Condensed Matter 34, 475802 (2022).

181 Theoretical study of topological properties of ferromagnetic pyrite CoS_2.
Robredo I, Schroter NBM, Reyes-Serrato A, Bergara A, de Juan F, Schoop LM, and Vergniory MG.
Journal of Physics D-Applied Physics 55, 304004 (2022).

182 The 2022 magneto-optics roadmap.
Kimel A, Zvezdin A, Sharma S, Shallcross S, de Sousa N, Garcia-Martin A, Salvan G, Hamrle J, Stejskal O, McCord J, et al.
Journal of Physics D-Applied Physics 55, 463003 (2022).

183 Sub- and supercritical hydrothermal route for the synthesis of xonotlite nanofibers for application to green concrete materials.
Musumeci V, Camacho PS, Xu K, Monteiro PJM, Dolado JS, and Aymonier C.
Journal of Supercritical Fluids 184, 105583 (2022).

184 A molecular dynamics study of N-A-S-H gel with various Si/Al ratios.
Chen Y, Dolado JS, Li ZM, Yin SH, Yu QJ, Kostiuchenko A, and Ye G.
Journal of the American Ceramic Sociey 105, 6462 (2022).

185 Structure matters: asymmetric CO oxidation at Rh steps with different atomic packing.
Garcia-Martinez F, Raemisch L, Ali K, Waluyo I, Bodero RC, Pfaff S, Villar-Garcia IJ, Walter AL, Hunt A, Perez-Dieste V, et al.
Journal of the American Chemical Society 144, 1536 (2022).

186 Solid-state pathway control via reaction-directing heteroatoms: ordered pyridazine nanothreads through selective cycloaddition.
Dunning SG, Zhu L, Chen B, Chariton S, Prakapenka VB, Somayazulu M, and Strobel TA.
Journal of the American Chemical Society 144, 2073 (2022).

187 Steric hindrance of NH_3 diffusion on Pt(111) by Co-adsorbed O-atoms.
Borodin D, Galparsoro O, Rahinov I, Fingerhut J, Schwarzer M, Horandl S, Auerbach DJ, Kandratsenka A, Schwarzer D, Kitsopoulos TN, and Wodtke AM.
Journal of the American Chemical Society 144, 21791 (2022).

188 Chemisorption-induced formation of biphenylene dimer on Ag(111).
Zeng Z, Guo D, Wang T, Chen Q, Matej A, Huang J, Han D, Xu Q, Zhao A, Jelinek P, et al.
Journal of the American Chemical Society 144, 723 (2022).

189 Phenanthrene-extended phenazine dication: an electrochromic conformational switch presenting dual reactivity.
Dosso J, Bartolomei B, Demitri N, Cossio FP, and Prato M.
Journal of the American Chemical Society 144, 7295 (2022).

190 Generation and characterization of the charge-transferred diradical complex $CaCO_2$ with an open-shell singlet ground state.
Zhou YY, Pan S, Dong XL, Wang LN, Zhou MF, and Frenking G.
Journal of the American Chemical Society 144, 8355 (2022).

191 Theoretical studies of furan and thiophene nanothreads: structures, cycloaddition barriers, and activation volumes.
Chen B, Crespi VH, and Hoffmann R.
Journal of the American Chemical Society 144, 9044 (2022).

192 Preparation, supramolecular organization, and on-surface reactivity of enantiopure subphthalocyanines: from bulk to 2D-polymerization.
Labella J, Lavarda G, Hernandez-Lopez L, Aguilar-Galindo F, Diaz-Tendero S, Lobo-Checa J, and Torres T.
Journal of the American Chemical Sopciety 144, 16579 (2022).

193 Aza-triangulene: on-surface synthesis and electronic and magnetic properties.
Wang T, Berdonces-Layunta A, Friedrich N, Vilas-Varela M, Calupitan JP, Pascual JI, Pena D, Casanova D, Corso M, and de Oteyza DG.
Journal of the American Chemical Society 144, 4522 (2022).

194 Twisted polaritonic crystals in thin van der Waals slabs.
Capote-Robayna N, Matveeva OG, Volkov VS, Alonso-Gonzalez P, and Nikitin AY.
Laser & Photonics Reviews 16, 2200428 (2022).

195 Disentangling component dynamics in an all-polymer nanocomposite based on single-chain nanoparticles by quasielastic neutron scattering.
Maiz J, Verde-Sesto E, Asenjo-Sanz I, Mangin-Thro L, Frick B, Pomposo JA, Arbe A, and Colmenero J.
Macromolecules 55, 2320 (2022).

196 Validity of effective potentials in crowded solutions of linear and ring polymers with reversible bonds.
Paciolla M, Likos CN, and Moreno AJ.
Macromolecules 55, 2659 (2022).

197 Disentangling the calorimetric glass-transition trace in polymer/oligomer mixtures from the modeling of dielectric relaxation and the input of small-angle neutron scattering.
Shafqat N, Alegria A, Arbe A, Malicki N, Dronet S, Porcar L, and Colmenero J.
Macromolecules 55, 7614 (2022).

198 Unveiling the hidden entropy in $ZnFe_2O_4$.
Cobos MA, Hernando A, Marco JF, Puente-Orench I, Jimenez JA, Llorente I, Garcia-Escorial A, and de la Presa P.
Materials 15, 1198 (2022).

199 Hardening and fresh state behaviour of ternary cement for marine environments: modification through nanoadditives.
Corro AM, Perlot C, Latapie E, and Cerveny S.
Materials 15, 1938 (2022).

200 Role of Eu^{2+} and Dy^{3+} concentration in the persistent luminescence of $Sr_2MgSi_2O_7$ glass-ceramics.
Fernandez-Rodriguez L, Balda R, Fernandez J, Duran A, and Pascual MJ.
Materials 15, 3068 (2022).

201 Ferrimagnetic clusters as the origin of anomalous Curie-Weiss behavior in $ZnFe_2O_4$ antiferromagnetic susceptibility.
Hernando A, Cobos MA, Jimenez JA, Llorente I, Garcia-Escorial A, and de la Presa, P.
Materials 15, 4789 (2022).

202 Thermal energy storage (TES) prototype based on geopolymer concrete for high-temperature applications.
Rahjoo M, Goracci G, Gaitero JJ, Martauz P, Rojas E, and Dolado JS.
Materials 15, 7086 (2022).

203 Correlations between helicity and optical losses within general electromagnetic scattering theory.
Lasa-Alonso J, Olmos-Trigo J, Garcia-Etxarri A, and Molina-Terriza G.
Materials Advances 3, 4179 (2022).

204 Oxygen non-stoichiometry and phase decomposition of double perovskite-like molybdates $Sr_2MMoO_{6-\delta}$, where M = Mn, Co, and Ni.
Tolstov KS, Politov BV, Zhukov VP, Chulkov EV, and Kozhevnikov VL.
Materials Letter 316, 132039 (2022).

205 Synthesis, structural and spectral characteristics of $Cd_3O_2SO_4$.
Krasil'nikov VN, Tyutyunnik AP, Zhukov VP, Baklanova IV, Reznitskikh OG, and Chulkov V.
Materials Today Communications 30, 103215 (2022).

206 Heretical thoughts about the present understanding and description of the chemical bond.
Frenking G.
Molecular Physics e2110168 (2022).

207 Sandwich, triple-decker and other sandwich-like complexes of cyclopentadienyl anions with lithium or sodium cations.
Grabowski SJ, and Parra RD.
Molecules 27, 6269 (2022).

208 Thermal conductivity of solid triphenyl phosphite.
Krivchikov A, Andersson O, Korolyuk O, and Kryvchikov O.
Molecules 27, 8399 (2022).

209 Subhalo abundance matching through the lens of a hydrodynamical simulation.
Favole G, Montero-Dorta AD, Artale MC, Contreras S, Zehavi I, and Xu XJ.
Monthly Notices of the Royal Astronomical Society 509, 1614 (2022).

210 Simulating the complexity of the dark matter sheet - II. Halo and subhalo mass functions for non-cold dark matter models.
Stucker J, Angulo RE, Hahn O, and White SDM.
Monthly Notices of the Royal Astronomical Society 509, 1703 (2022).

211 Redshift-space effects in voids and their impact on cosmological tests - II. The void-galaxy cross-correlation function.
Correa CM, Paz DJ, Padilla ND, Sanchez AG, Ruiz AN, and Angulo RE.
Monthly Notices of the Royal Astronomical Society 509, 1871 (2022).

212 Supermassive black holes in cosmological simulations - II:
the AGN population and predictions for upcoming x-ray missions.
Habouzit M, Somerville RS, Li Y, Genel S, Aird J, Angles-Alcazar D, Dave R, Georgiev IY, McAlpine S, Rosas-Guevara Y, et al
Monthly Notices of the Royal Astronomical Society 509, 3015 (2022).

213 Massive black hole evolution models confronting the n-Hz amplitude
of the stochastic gravitational wave background.
Izquierdo-Villalba D, Sesana A, Bonoli S, and Colpi M.
Monthly Notices of the Royal Astronomical Society 509, 3488 (2022).

214 Non-universality of the mass function: dependence on the growth rate
and power spectrum shape.
Ondaro-Mallea L, Angulo RE, Zennaro M, Contreras S, and Arico G.
Monthly Notices of the Royal Astronomical Society 509, 6077 (2022).

215 Star cluster ecology: revisiting the origin of iron and age complex clusters.
de Bastian N, and Pfeffer J.
Monthly Notices of the Royal Astronomical Society 509, 614 (2022).

216 zELDA: fitting Lyman alpha line profiles using deep learning.
Gurung-Lopez S, Gronke M, Saito S, Bonoli S, and Orsi AA.
Monthly Notices of the Royal Astronomical Society 510, 4525 (2022).

217 UNITSIM-galaxies: data release and clustering of emission-line galaxies.
Knebe A, Lopez-Cano D, Avila S, Favole G, Stevens ARH, Gonzalez-Perez V, Reyes-Peraza G, Yepes G, Chuang CH, and Kitaura FS.
Monthly Notices of the Royal Astronomical Society 510, 5392 (2022).

218 The physics governing the upper truncation mass of the globular cluster mass function.
Hughes ME, Pfeffer JL, Bastian N, Martig M, Kruijssen JMD, Crain RA,
Reina-Campos M, and Trujillo-Gomez S.
Monthly Notices of the Royal Astronomical Society 510, 6190 (2022).

219 The evolution of the oxygen abundance gradients in star-forming galaxies
in the EAGLE simulations.
Tissera PB, Rosas-Guevara Y, Sillero E, Pedrosa SE, Theuns T, and Bignone L.
Monthly Notices of the Royal Astronomical Society 511, 1667 (2022).

220 A black hole detected in the young massive LMC cluster NGC 1850.
Saracino S, Kamann S, Guarcello MG, Usher C, Bastian N, Cabrera-Ziri I, Gieles M, Dreizler S, Da Costa GS , Husser TO, and Henault-Brunet V.
Monthly Notices of the Royal Astronomical Society 511, 2914 (2022).

221 Non-halo structures and their effects on gravitational lensing.
Richardson TRG, Stucker J, Angulo RE, and Hahn O.
Monthly Notices of the Royal Astronomical Society 511, 6019 (2022).

222 The cosmic web connection to the dark matter halo distribution through gravity.
Kitaura FS, Balaguera-Antolinez A, Sinigaglia F, and Pellejero-Ibanez M.
Monthly Notices of the Royal Astronomical Society 512, 2245 (2022).

223 The evolution of the barred galaxy population in the TNG50 simulation.
Rosas-Guevara Y, Bonoli S, Dotti M, Izquierdo-Villalba D, Lupi A, Zana T, Bonetti M, Nelson D, Springel V, Hernquist L, and Vogelsberger M.
Monthly Notices of the Royal Astronomical Society 512, 5339 (2022).

224 Radial distributions of globular clusters trace their host dark matter halo:
insights from the E-MOSAICS simulations.
Reina-Campos M, Trujillo-Gomez S, Deason AJ, Kruijssen JMD, Pfeffer JL, Crain RA,
Bastian N, and Hughes ME.
Monthly Notices of the Royal Astronomical Society 513, 3925 (2022).

225 Disc instability and bar formation: view from the illustrisTNG simulations.
Izquierdo-Villalba D, Bonoli S, Rosas-Guevara Y, Springel V, White SDM, Zana T, Dotti M, Spinoso D, Bonetti M, and Lupi A.
Monthly Notices of the Royal Astronomical Society 514, 1006 (2022).

226 Modelling galaxy clustering in redshift space with a Lagrangian bias formalism
and N-body simulations.
Pellejero-Ibanez M, Stucker J, Angulo RE, Zennaro M, Contreras S, and Arico G.
Monthly Notices of the Royal Astronomical Society 514, 3993 (2022).

227 Priors on Lagrangian bias parameters from galaxy formation modelling.
Zennaro M, Angulo RE, Contreras S, Pellejero-Ibanez M, and Maion F.
Monthly Notices of the Royal Astronomical Society 514, 5443 (2022).

228 Morphological decomposition of TNG50 galaxies: methodology and catalogue.
Zana T, Lupi A, Bonetti M, Dotti M, Rosas-Guevara Y, Izquierdo-Villalba D, Bonoli S,
Hernquist L, and Nelson D.
Monthly Notices of the Royal Astronomical Society 515, 1524 (2022).

229 Machine learning synthetic spectra for probabilistic redshift estimation: SYTH-Z.
Ramachandra N, Chaves-Montero J, Alarcon A, Fadikar A, Habib S, and Heitmann K.
Monthly Notices of the Royal Astronomical Society 515, 1927 (2022).

230 Understanding the 'feeble giant' crater II with tidally stretched wave dark matter.
Pozo A, Broadhurst T, Emami R, and Smoot G.
Monthly Notices of the Royal Astronomical Society 515, 2624 (2022).

231 S-PLUS: exploring wide field properties of multiple populations in galactic globular clusters
at different metallicities.
Hartmann EA, Bonatto CJ, Chies-Santos AL, Alonso-Garcia J, Bastian N, Overzier R, Schoenell W, Coelho PRT, Branco V, Kanaan A, et al.
Monthly Notices of the Royal Astronomical Society 515, 4191 (2022).

232 Milky way-like galaxies: stellar population properties of dynamically defined discs, bulges and stellar haloes.
Ortega-Martinez S, Obreja A, Dominguez-Tenreiro R, Pedrosa SE, Rosas-Guevara Y, and Tissera PB.
Monthly Notices of the Royal Astronomical Society 516, 197 (2022).

233 Testing the key role of the stellar mass-halo mass relation in galaxy merger rates and morphologies via DECODE, a novel discrete statistical sEmi-empiriCal mODEl.
Fu H, Shankar F, Ayromlou M, Dickson M, Koutsouridou I, Rosas-Guevara Y, Marsden C, Brocklebank K, Bernardi M, Shiamtanis N, et al.
Monthly Notices of the Royal Astronomical Society 516, 3206 (2022).

234 The cosmology dependence of the concentration-mass-redshift relation.
Lopez-Cano D, Angulo RE, Ludlow AD, Zennaro M, Contreras S, Chaves-Montero J, and Arico G.
Monthly Notices of the Royal Astronomical Society 517, 2000 (2022).

235 Revealing the properties of void galaxies and their assembly using the EAGLE simulation.
Rosas-Guevara Y, Tissera P, Lagos CD, Paillas E, and Padilla N.
Monthly Notices of the Royal Astronomical Society 517, 712 (2022).

236 One-dimensional heterostructure: The selective decoration of single-walled carbon nanotube tins with metallic nanoparticles.
Castillo AED, Soriano ML, Grzelczak M, Quintana M, and Prato M.
MRS Bulletin 47, 675 (2022).

237 Magnetic interactions between radical pairs in chiral graphene nanoribbons.
Wang T, Sanz S, Castro-Esteban J, Lawrence J, Berdonces-Layunta A, Mohammed MSG, Vilas-Varela M, Corso M, Pena D, Frederiksen T, and de Oteyza DG.
Nano Letters 22, 164 (2022).

238 Electron paramagnetic resonance of alkali metal atoms and dimers on ultrathin MgO.
Kovarik S, Robles R, Schlitz R, Seifert TS, Lorente N, Gambardella P, and Stepanow S.
Nano Letters 22, 4176 (2022).

239 Electrostatic interactions in twisted bilayer graphene.
Cea T, Pantaleon PA, Walet NR, and Guinea F.
Nano Materials Science 4, 27 (2022).

240 Efficient passivation of DY center in $CH_3NH_3PbBr_3$ by chlorine: quantum molecular dynamics.
Shi R, Fang WH, Vasenko AS, Long R, and Prezhdo OV.
Nano Research 15, 2112 (2022).

241 Superfluidity of dipolar excitons in a double layer of $\alpha - T_3$ with a mass term.
Berman OL, Gumbs G, Martins GP, and Fekete P.
Nanomaterials 12, 1437 (2022).

242 Skyrmion dynamics in a double-disk geometry under an electric current.
Castillo-Sepulveda S, Velez JA, Corona RM, Carvalho-Santos VL, Laroze D, and Altbir D.
Nanomaterials 12, 3086 (2022)

243 Skyrmion dynamics in a double-disk geometry under an electric current: part two.
Castillo-Sepulveda S, Velez JA, Corona RM, Carvalho-Santos VL, Laroze D, and Altbir D.
Nanomaterials 12, 3793 (2022).

244 Electrical conductive properties of 3D-printed concrete composite with carbon nanofibers.
Goracci G, Salgado DM, Gaitero JJ, and Dolado JS.
Nanomaterials 12, 3939 (2022).

245 Influence of tartrate ligand coordination over luminescence properties of chiral lanthanide-based metal-organic frameworks.
Huizi-Rayo U, Gastearena X, Ortuno AM, Cuerva JM, Rodriguez-Dieguez A, Garcia JA, Ugalde J, Seco JM, San Sebastian E, and Cepeda J.
Nanomaterials 12, 3999 (2022).

246 One-step theory view on photoelectron diffraction: application to graphene.
Krasovskii E.
Nanomaterials 12, 4040 (2022).

247 Revising quantum optical phenomena in adatoms coupled to graphene nanoantennas.
Kosik M, Muller MM, Slowik K, Bryant G, Ayuela A, Rockstuhl C, and Pelc M.
Nanophotonics 11, 3281 (2022).

248 Rhombohedral trilayer graphene is more stable than its Bernal counterpart.
Guerrero-Aviles R, Pelc M, Geisenhof FR, Weitz RT, and Ayuela A.
Nanoscale 14, 16295 (2022).

249 Empowering non-covalent hydrogen, halogen, and $[S\text{-}N]_2$ bonds in synergistic molecular assemblies on Au(111).
Barragan A, Lois S, Sarasola A, and Vitali L.
Nanoscale 14, 17895 (2022).

250 On-surface synthesis of Mn-phthalocyanines with optically active ligands.
Dominguez-Celorrio A, Garcia-Fernandez C, Quiroga S, Koval P, Langlais V, Pena D, Sanchez-Portal D, Serrate D, and Lobo-Checa J.
Nanoscale 14, 8069 (2022).

251 A highly magnified star at redshift 6.2.
Welch B, Coe D, Diego JM, Zitrin A, Zackrisson E, Dimauro P, Jimenez-Teja Y, Kelly P, Mahler G, Oguri M, et al.
Nature 603, 815 (2022).

252 Catalogue of flat-band stoichiometric materials.
Regnault N, Xu YF, Li MR, Ma DS, Jovanovic M, Yazdani A, Parkin SSP, Felser C, Schoop LM, Ong NP, et al.
Nature 603, 824 (2022).

253 Switchable chiral transport in charge-ordered kagome metal CsV_3Sb_5.
Guo CY, Putzke C, Konyzheva S, Huang XW, Gutierrez-Amigo M, Errea I, Chen D, Vergniory MG, Felser C, Fischer MH, et al.
Nature 611, 461 (2022).

254 Shock cooling of a red-supergiant supernova at redshift 3 in lensed images.
Chen WL, Kelly PL, Oguri M, Broadhurst TJ, Diego JM, Emami N, Filippenko AV, Treu TL, and Zitrin A.
Nature 611, 7935 (2022).

255 Circumventing the stability problems of graphene nanoribbon zigzag edges.
Lawrence J, Berdonces-Layunta A, Edalatmanesh S, Castro-Esteban J, Wang T, Jimenez-Martin A, de la Torre B, Castrillo-Bodero R, Angulo-Portugal P, Mohammed MSG, et al.
Nature Chemistry 14, 1451 (2022).

256 Real-space nanoimaging of THz polaritons in the topological insulator Bi_2Se_3.
Chen S, Bylinkin A, Wang ZTY, Schnell M, Chandan G, Li PN, Nikitin AY, Law S, and Hillenbrand R.
Nature Communications 13, 1374 (2022).

257 Radiationless mechanism of UV deactivation by cuticle phenolics in plants.
Moreno AG, de Cozar A, Prieto P, Dominguez E, and Heredia A.
Nature Communications 13, 1786 (2022).

258 Superconducting spintronic tunnel diode.
Strambini E, Spies M, Ligato N, Ilic S, Rouco M, Gonzalez-Orellana C, Ilyn M, Rogero C, Bergeret FS, and Moodera JS.
Nature Communications 13, 2431 (2022).

259 Magnons and magnetic fluctuations in atomically thin $MnBi_2Te_4$.
Lujan D, Choe J, Rodriguez-Vega M, Ye ZP, Leonardo A, Nunley TN, Chang LJ, Lee SF, Yan JQ, and Fiete GA.
Nature Communications 13, 2527 (2022).

260 Sustainable oxygen evolution electrocatalysis in aqueous 1 M H_2SO_4 with earth abundant nanostructured Co_3O_4.
Yu JH, Garces-Pineda FA, Gonzalez-Cobos J, Pena-Diaz M, Rogero C, Gimenez S, Spadaro MC, Arbiol J, Barja S, and Galan-Mascaros JR.
Nature Communications 13, 4341 (2022).

261 Topological zero-dimensional defect and flux states in three-dimensional insulators.
Schindler F, Tsirkin SS, Neupert T, Bernevig BA, and Wieder BJ.
Nature Communications 13, 5791 (2022).

262 All-optical control of spin in a 2D van der Waals magnet.
Dabrowski M, Guo S, Strungaru M, Keatley PS, Withers F, Santos EJG, and Hicken RJ.
Nature Communications 13, 5976 (2022).

263 Stabilization of three-dimensional charge order through interplanar orbital hybridization in $Pr_xY_{1-x}Ba_2Cu_3O_{6+\delta}$.
Ruiz A, Gunn B, Lu Yi, Sasmal K, Moir CM, Basak R, Huang H, Lee JS, Rodolakis F, Boyle TJ, et al.
Nature Communications 13, 6197 (2022).

264 Remote near-field spectroscopy of vibrational strong coupling between organic molecules and phononic nanoresonators.
Dolado I, Maciel-Escudero C, Nikulina E, Modin E, Calavalle F, Chen S, Bylinkin A, Alfaro-Mozaz FJ, Li JH, Edgar JH, et al.
Nature Communications 13, 6850 (2022).

265 Breaking through the Mermin-Wagner limit in 2D van der Waals magnets.
Jenkins S, Rozsa L, Atxitia U, Evans RFL, Novoselov KS, and Santos EJG.
Nature Communications 13, 6917 (2022).

266 Ba^{+2} ion trapping using organic submonolayer for ultra-low background neutrinoless double beta detector.
Herrero-Gomez P, Calupitan JP, Ilyn M, Berdonces-Layunta A, Wang T, de Oteyza DG, Corso M, Gonzalez-Moreno R, Rivilla I, Aparicio B, et al.
Nature Communications 13, 7741 (2022).

267 Exchange scaling of ultrafast angular momentum transfer in 4f antiferromagnets.
Windsor YW, Lee SE, Zahn D, Borisov V, Thonig D, Kliemt K, Ernst A, Schussler-Langeheine C, Pontius N, Staub U, et al.
Nature Materials 21, 514 (2022).

268 Topological semimetal driven by strong correlations and crystalline symmetry.
Chen L, Chandan S, Haoyu H, Vergniory MG, Grefe SE, Fischer L, Yan X, Eguchi G, Prokofiev A, Paschen S, et al.
Nature Physics 18, 1341 (2022).

269 General construction and topological classification of crystalline flat bands.
Calugaru D, Chew A, Elcoro L, Xu YF, Regnault N, Song ZD, and Bernevig BA.
Nature Physics 18, 185 (2022).

270 Quasi-symmetry-protected topology in a semi-metal.
Guo CY, Hu LH, Putzke C, Diaz J, Huang XW, Manna K, Fan FR, Shekhar C, Sun Y, Felser C, et al.
Nature Physics 18, 813 (2022).

271 Topological materials discovery from crystal symmetry.
Wieder BJ, Bradlyn B, Cano J, Wang ZJ, Vergniory MG, Elcoro L, Soluyanov AA, Felser C, Neupert T, Regnault N, and Bernevig BA.
Nature Reviews Materials 7, 196 (2022).

272 Superconductivity, superfluidity and quantum geometry in twisted multilayer systems.
Torma P, Peotta S, and Bernevig BA.
Nature Reviews Physics 4, 528 (2022).

273 Rashba-like physics in condensed matter.
Bihlmayer G, Noel P, Vyalikh DV, Chulkov EV, and Manchon A.
Nature Reviews Physics 4, 642 (2022).

274 Egocentric vision-based action recognition: a survey.
Nunez-Marcos A, Azkune G, and Arganda-Carreras I.
Neurocomputing 472, 175 (2022).

275 Stable deep neural network architectures for mitochondria segmentation on electron microscopy volumes.
Franco-Barranco D, Munoz-Barrutia A, and Arganda-Carreras I.
Neuroinformatics 20, 437 (2022).

276 Spatial aspects of spin polarization of structurally split surface states in thin films with magnetic exchange and spin-orbit interaction.
Nechaev IA, and Krasovskii EE.
New Journal of Physics 24, 013021 (2022).

277 Topological lifshitz transitions, orbital currents, and interactions in low-dimensional Fermi gases in synthetic gauge fields.
Huang CH, Tezuka M, and Cazalilla MA.
New Journal of Physics 24, 033043 (2022).

278 Ultrafast laser-driven topological spin textures on a 2D magnet.
Strungaru M, Augustin M, and Santos EJG.
NPJ Computational Materials 8, 169 (2022).

279 An atomistic approach for the structural and electronic properties of twisted bilayer graphene-boron nitride heterostructures.
Long M, Pantaleon PA, Zhan Z, Guinea F, Silva-Guillen JA, and Yuan S.
NPJ Computational Materials 8, 73 (2022).

280 Native point defects and their implications for the Dirac point gap at $MnBi_2Te_4$(0001).
de Garnica M, Otrokov MM, Aguilar PC, Klimovskikh II, Estyunin D, Aliev ZS, Amiraslanov IR, Abdullayev NA, Zverev VN, Babanly MB, et al.
NPJ Quantum Materials 7, 7 (2022).

281 The dynamics of ions on phased radio-frequency carpets in high pressure gases and application for barium tagging in xenon gas time projection chambers.
Jones BJP, Raymond A, Woodruff K, Byrnes N, Denisenko AA, Foss FW, Navarro K, Nygren DR, Vuong TT, Adams C, et al.
Nuclear Instruments and Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment 1039, 167000 (2022).

282 Rare-earth doped transparent oxyfluoride glass-ceramics: processing is the key [invited].
Cruz ME, Sedano M, Castro Y, Pascual MJ, Fernandez J, Balda R, and Duran A.
Optical Materials Express 12, 3493 (2022).

283 Bandwidth control of the biphoton wavefunction exploiting spatio-temporal correlations.
Varga JJM, Lasa-Alonso J, Molezuelas-Ferreras M, Tischler N, and Molina-Terriza G.
Optics Communications 504, 127461 (2022).

284 Spectro-temporal behavior of dye-based solid-state random lasers under picosecond pumping regime.
Iparraguirre I, Azkargorta J, Garcia-Revilla S, Fernandez J, and Balda R.
Optics Express 30, 9674 (2022).

285 Quantum surface effects in the electromagnetic coupling between a quantum emitter and a plasmonic nanoantenna: time-dependent density functional theory vs. semiclassical Feibelman approach.
Babaze A, Ogando E, Stamatopoulou PE, Tserkezis C, Mortensen NA, Aizpurua J, Borisov AG, and Esteban R.
Optics Express 30, 21159 (2022).

286 Spectro-temporal behavior of dye-based solid-state random lasers under picosecond pumping regime: part II
Iparraguirre I, Azkargorta J, Garcia-Revilla S, Fernandez J, and Balda R.
Optics Express 30, 26655 (2022).

287 Broadening the absorption bandwidth based on heavily doped semiconductor nanostructures.
Goncharenko AV, Fitio V, and Silkin V.
Optics Express 30, 36622 (2022).

288 Knolker iron catalysts for hydrogenation revisited: a nonspectator solvent and fine-tuning.
Gimferrer M, Joly N, Escayola S, Vinas E, Gaillard S, Sola M, Renaud JL, Salvador P, and Poater A.
Organometallics 41, 1204 (2022).

289 Photoactive platinum(II) azopyridine complexes(dagger).
Farley SJ, Salassa L, Pizarro AM, and Sadler PJ.
Photochemistry and Photobiology 98, 92 (2022).

290 Effective conductivity of random composites with shape-distributed near-spherical inclusions.
Goncharenko AV, Venger EF, and Pinchuk AO.
Physica B-Condensed Matter 639, 413943 (2022).

291 Detecting magnetic permeability and electrical conductivity fluctuations in metallic ferromagnetic sheets through the shielding effect.
Hernando A, Giacomone F , Vinolas J, Garcia MA, Galvez F, Castellanos A, de Hoyos A, and Cerracin A.
Physica Satus Solidi B-Basic Solid State Physics 259, 2100446 (2022).

292 The kinks, the solitons and the shocks in series-connected discrete Josephson transmission lines.
Kogan E.
Physica Satus Solidi B-Basic Solid State Physics 259, 2200160 (2022).

293 Electron-phonon coupling and superconductivity in a 2D Tl-Pb compound on Si(111).
Sklyadneva IY, Heid R, Echenique PM, and Chulkov EV.
Physical Chemistry Chemical Physics 24, 10140 (2022).

294 Semi-empirical and linear-scaling DFT methods to characterize duplex DNA and G-quadruplexes in the presence of interacting small molecules.
de Luzuriaga IO, Elleuchi S, Jarraya K, Artacho E, Lopez X, and Gil A.
Physical Chemistry Chemical Physics 24, 11510 (2022).

295 On surface chemical reactions of free-base and titanyl porphyrins with r-TiO_2(110): a unified picture.
Schio L, Forrer D, Casarin M, Goldoni A, Rogero C, Vittadini A, and Floreano L.
Physical Chemistry Chemical Physics 24, 12719 (2022).

296 Clarifying notes on the bonding analysis adopted by the energy decomposition analysis.
Bickelhaupt FM, Guerra CF, Mitoraj M, Sagan F, Michalak A, Pan S, and Frenking G.
Physical Chemistry Chemical Physics 24, 15726 (2022).

297 How to capture C_2O_2: structures and bonding of neutral and charged complexes [(NHC)-C_2O_2-(NHC)]^q (NHC = N-heterocyclic carbene; q=0, 1+, 2+).
Ding CX, Yao L, Zhao LL, and Frenking G.
Physical Chemistry Chemical Physics 24, 16732 (2022).

298 Atom-surface scattering in the classical multiphonon regime.
Manson JR, and Miret-Artes S.
Physical Chemistry Chemical Physics 24, 16942 (2022).

299 Impact of the energy dispersion anisotropy on the plasmonic structure in a two-dimensional electron system.
Muniain U, and Silkin VM.
Physical Chemistry Chemical Physics 24, 17885 (2022).

300 Variation of bending rigidity with material density: bilayer silica with nanoscale holes.
Tomterud M, Eder SD, Buchner C, Heyde M, Freund HJ, Manson JR, and Holst B.
Physical Chemistry Chemical Physics 24, 17941 (2022).

301 Time-dependent density functional theory calculations of electronic friction in non-homogeneous media.
Koval NE, Sanchez-Portal D, Borisov AG, and Diez Muino R.
Physical Chemistry Chemical Physics 24, 20239 (2022).

302 The role of high-energy phonons in electron-phonon interaction at conducting surfaces with helium-atom scattering.
Benedek G, Manson JR, and Miret-Artes S.
Physical Chemistry Chemical Physics 24, 23135 (2022).

303 Unravelling the binding affinity and selectivity of molybdenum(II) phenanthroline complexes with DNA G-quadruplexes by using linear-scaling DFT studies. The important role of ancillary ligands.
de Luzuriaga IO, Sanchez-Gonzalez A, Synoradzki W, Lopez X, and Gil A.
Physical Chemistry Chemical Physics 24, 25918 (2022).

304 New trends and challenges in surface phenomena, carbon nanostructures and helium droplets—Festschrift for Giorgio Benedek.
Bernasconi M, Muino RD, Echenique PM, Manson JR, Miret-Artes S, and Toennies JP.
Physical Chemistry Chemical Physics 24, 28103 (2022).

305 Giorgio Benedek: an extraordinary scientist and cultured gentleman.
Bernasconi M, Muino RD, Echenique PM, Manson JR, Miret-Artes S, and Toennies JP.
Physical Chemistry Chemical Physics 24, 28105 (2022).

306 Excited state dynamics and conjugation effects of the photoisomerization reactions of dihydroazulene.
Hillers-Bendtsen AE, Kjeldal FO, Ree N, Matito E, and Mikkelsen KV.
Physical Chemistry Chemical Physics 24, 28934 (2022).

307 Three-centre electron sharing indices (3c-ESIs) as a tool to differentiate among (an)agostic interactions and hydrogen bonds in transition metal complexes.
Garcia-Rodeja Y, Feixas F, Matito E, and Sola M.
Physical Chemistry Chemical Physics 24, 29333 (2022).

308 Surface dynamics on submonolayer Pb/Cu(001) surfaces.
Borisova SD, Eremeev SV, Rusina GG, and Chulkov EV.
Physical Chemistry Chemical Physics 24, 5164 (2022).

309 Flavin-mediated photoactivation of Pt(IV) anticancer complexes: computational insights on the catalytic mechanism.
Scoditti S, Dabbish E, Pieslinger GE, Rezabal E, Lopez X, Sicilia E, and Salassa L.
Physical Chemistry Chemical Physics 24, 5323 (2022).

310 Generation of multiple triplet states in an orthogonal bodipy dimer: a breakthrough spectroscopic and theoretical approach.
Garcia-Moreno I, Postils V, Rebollar E, Ortiz MJ, Agarrabeitia AR, and Casanova D.
Physical Chemistry Chemical Physics 24, 5929 (2022).

311 Dark solitons in a trapped gas of long-range interacting bosons.
Beau M, del Campo A, Frantzeskakis DJ, Horikis TP, and Kevrekidis PG.
Physical Review A 105, 023323 (2022).

312 Entropy-based formulation of thermodynamics in arbitrary quantum evolution.
Alipour S, Rezakhani AT, Chenu A, del Campo A, and Ala-Nissila T.
Physical Review A 105, L040201(2022).

313 Dynamical stabilization by vacuum fluctuations in a cavity: resonant electron scattering in the ultrastrong light-matter coupling regime.
Zezyulin DA, Kolodny SA, Kibis OV, Tokatly I, and Iorsh IV.
Physical Review A 106, 043708 (2022).

314 Tunable near-field radiative effect in a T_d–WTe_2 single layer.
Zhou CL, Torbatian Z, Wu XH, Zhang Y, Yi HL, and Novko D.
Physical Review Applied 17, 014044 (2022).

315 Current rectification in junctions with spin-split superconductors.
Ilic S, Virtanen P, Heikkila TT, and Bergeret FS.
Physical Review Applied 17, 034049 (2022).

316 Room-temperature van der Waals perpendicular ferromagnet through interlayer magnetic coupling.
Cao Y, Zhang XM, Zhang XP, Yan FG, Wang Z, Zhu WK, Tan H, Golovach VN, Zheng HZ, and Wang KY.
Physical Review Applied 17, L051001 (2022).

317 Entangling nuclear spins in distant quantum dots via an electron bus.
Bello M, Benito M, Schuetz MJA, Platero G, and Giedke G.
Physical Review Applied 18, 014009 (2022).

318 Helicity conservation for mie optical cavities.
Olmos-Trigo J, and Zambrana-Puyalto X.
Physical Review Applied 18, 044007 (2022).

319 Quantum annealing sampling with a bias field.
Grass T.
Physical Review Applied 18, 044036 (2022).

320 Hybrid photonic-plasmonic cavity design for very large purcell factors at telecommunication wavelengths.
Barreda A, Mercade L, Zapata-Herrera M, Aizpurua J, and Martinez A.
Physical Review Applied 18, 044066 (2022).

321 Calculations of in-gap states of ferromagnetic spin chains on s-wave wide-band superconductors.
Mier C, Choi DJ, and Lorente N.
Physical Review B 104, 245415 (2022).

322 Superconducting LaP_2H_2 with graphenelike phosphorus layers.
de Li X, Zhang XH, Bergara A, Gao GY, Liu Y, and Yang GC.
Physical Review B 105, 024504 (2022).

323 Exact quantum scars in the chiral nonlinear luttinger liquid.
Schindler F, Regnault N, and Bernevig BA.
Physical Review B 105, 035146 (2022).

324 Revisiting the physical origin and nature of surface states in inverted-band semiconductors.
Khaetskii A, Golovach V, and Kiefer A.
Physical Review B 105, 035305 (2022).

325 Adsorption and dissociation of diatomic molecules on monolayer 1H-$MoSe_2$.
Bombin R, Alducin M, and Juaristi JI.
Physical Review B 105, 035404 (2022).

326 Multidimensional multiphoton momentum microscopy of the anisotropic Ag(110) surface.
de Li AD, Reutzel M, Wang ZH, Schmitt D, Keunecke M, Bennecke W, Jansen GSM, Steil D, Steil S, Novko D, et al.
Physical Review B 105, 075105 (2022).

327 Superconductivity from repulsive interactions in rhombohedral trilayer graphene: a Kohn-Luttinger-like mechanism.
Cea T, Pantaleon PA, Phong VT, and Guinea F.
Physical Review B 105, 075432 (2022).

328 Semilocal approximations to the Kohn-Sham exchange potential as applied to a metal surface.
Horowitz CM, Proetto CR, and Pitarke JM.
Physical Review B 105, 085149 (2022).

329 Corner modes of the breathing kagome lattice: origin and robustness.
Herrera MAJ, Kempkes SN, de Paz MB, Garcia-Etxarri A, Swart I, Smith CM, and Bercioux D.
Physical Review B 105, 085411 (2022).

330 Unconventional superconductivity due to interband polarization.
Crepel V, Cea T, Fu L, and Guinea F.
Physical Review B 105, 094506 (2022).

331 Optically modulated tunneling current of dressed electrons in graphene and a dice lattice.
Iurov A, Zhemchuzhna L, Gumbs G, Huang DH, and Fekete P.
Physical Review B 105, 115309 (2022),

332 Topology invisible to eigenvalues in obstructed atomic insulators.
Cano J, Elcoro L, Aroyo MI, Bernevig A, and Bradlyn B.
Physical Review B 105, 125115 (2022).

333 Scattering effects from neighboring atoms in core-level WSe_2 photoemission.
Ambrosio MJ, Plesiat E, Decleva P, Echenique PM, Muino RD, and Martin F.
Physical Review B 105, 125405 (2022).

334 Out-of-plane magnetic anisotropy in bulk ilmenite $CoTiO_3$.
Arruabarrena M, Leonardo A, Rodriguez-Vega M, Fiete GA, and Ayuela A.
Physical Review B 105, 144425 (2022).

335 Trions in twisted bilayer graphene.
Schindler F, Vafek O, and Bernevig BA.
Physical Review B 105, 155135 (2022).

336 Quasiparticle density of states and triplet correlations in superconductor/ferromagnetic-insulator structures across a sharp domain wall.
Hijano A, Golovach VN, and Bergeret FS.
Physical Review B 105, 174507 (2022).

337 Magnetic ordering and topology in Mn_2 Bi_2 Te_5 and Mn2 Sb_2 Te_5 van der Waals materials.
Eremee SV, Otrokov MM, Ernst A, and Chulkov EV.
Physical Review B 105, 195105 (2022).

338 Strain-driven chiral phonons in two-dimensional hexagonal materials.
Rostami H, Guinea F, and Cappelluti E.
Physical Review B 105, 195431 (2022).

339 Theory of proximity effect in s+p-wave superconductor junctions.
Tanaka Y, Kokkeler T, and Golubov A.
Physical Review B 105, 214512 (2022).

340 Nonlinear s model for disordered systems with intrinsic spin-orbit coupling.
Virtanen P, Bergeret FS, and Tokatly IV.
Physical Review B 105, 224517 (2022).

341 Local orbital formulation of the Floquet theory of projectile electronic stopping.
Famili M, Forcellini N, and Artacho E.
Physical Review B 105, 245139 (2022).

342 Yu-Shiba-Rusinov states in two-dimensional superconductors with arbitrary Fermi contours.
Ortuzar J, Trivini S, Alvarado M, Rouco M, Zaldivar J, Yeyati AL, Pascual JI, and Bergeret S.
Physical Review B 105, 245403 (2022).

343 Finite-temperature plasmons, damping, and collective behavior in the α–T_3 model.
Iurov A, Zhemchuzhna L, Gumbs G, Huang DH, Dahal D, and Abranyos Y.
Physical Review B 105, 245414 (2022).

344 Nodal-line driven anomalous susceptibility in ZrSiS.
Gudac B, Kriener M, Sharlai YV, Bosnar M, Orbanie F, Mikitik GP, Kimura A, Kokanovic I, and Novak M.
Physical Review B 105, L241115 (2022).

345 Enhanced superconductivity in CuH_2 monolayers.
Yan X, Ding SC, Zhang XH, Bergara A, Liu Y, Wang YC, Zhou XF, and Yang GC.
Physical Review B 106, 014514 (2022).

346 Revisiting flat band superconductivity: dependence on minimal quantum metric and band touchings.
Huhtinen KE, Herzog-Arbeitman J, Chew A, Bernevig BA, and Torma P.
Physical Review B 106, 014518 (2022).

347 Multiplet effects in the electronic correlation of one-dimensional magnetic transition metal oxides on metals.
Goikoetxea J, Friedrich C, Bihlmayer G, Blugel S, Arnau A, and Blanco-Rey M.
Physical Review B 106, 035130 (2022).

348 Nature of interfacial Dzyaloshinskii-Moriya interactions in graphene/Co/Pt(111) multilayer heterostructures.
Blanco-Rey M, Bihlmayer G, Arnau A, and Cerda JI.
Physical Review B 106, 064426 (2022).

349 Three-dimensional Fermi surfaces from charge order in layered CsV_3 Sb_5.
Huang XW, Guo CY, Putzke C, Gutierrez-Amigo M, Sun Y, Vergniory MG, Errea I, Chen D, Felser C, and Moll PJW.
Physical Review B 106, 064510 (2022).

350 Ab initio self-consistent many-body theory of polarons at all couplings.
Lafuente-Bartolome J, Lian C, Sio WH, Gurtubay IG, Eiguren A, and Giustino F.
Physical Review B 106, 075119 (2022).

351 Strain-induced collapse of Landau levels in real Weyl semimetals.
Lee YJ, Park CH, and Vozmediano MAH.
Physical Review B 106, 075125 (2022).

352 Converging tetrahedron method calculations for the nondissipative parts of spectral functions.
Ghim M, and Park CH.
Physical Review B 106, 075126 (2022).

353 Magnetic bloch theorem and reentrant flat bands in twisted bilayer graphene at 2π flux.
Herzog-Arbeitman J, Chew A, and Bernevig BA.
Physical Review B 106, 085140 (2022).

354 Skyrmion lattice hosted in synthetic antiferromagnets and helix modes.
Wang XG, Chotorlishivil L, Tatara G, Dyrdal A, Guo GH, Dugaev VK, Barnas J, Parkin SSP, and Ernst A.
Physical Review B 106, 104424 (2022).

355 Stopping and image forces acting on a charged particle moving near a graphene-Al_2 O_3-graphene heterostructure.
Kalinic A, Despoja V, Radovic I, Karbunar L, and Miskovic ZL.
Physical Review B 106, 115430 (2022).

356 Extrinsic spin-valley Hall effect and spin-relaxation anisotropy in magnetized and strained graphene.
Zhang XP.
Physical Review B 106, 115437 (2022).

357 Role of boundary conditions in the full counting statistics of topological defects after crossing a continuous phase transition.
Gomez-Ruiz FJ, Subires D, and del Campo A.
Physical Review B 106, 134302 (2022).

358 Impact of ionic quantum fluctuations on the thermodynamic stability and superconductivity of $LaBH_8$.
Belli F, and Errea I.
Physical Review B 106, 134509 (2022).

359 Crystal electric field and properties of 4f magnetic moments at the surface of the rare-earth compound $TbRh_2$ Si_2.
Tarasov AV, Glazkova D, Schulz S, Poelchen G, Kliemt K, Kraiker A, Muntwiler M, Laubschat C, Generalov A, Polley C, Krellner C, Vyalikh DV, and Usachov DY.
Physical Review B 106, 155136 (2022).

360 Berry curvature induced anomalous hall conductivity in the magnetic topological oxide double perovskite Sr_2 $FeMoO_6$.
Chakraborty T, Samanta K, Guin SN, Noky J, Robredo I, Prasad S, Kuebler J, Shekhar C, Vergniory MG, and Felser C.
Physical Review B 106, 155141 (2022).

361 Charge-to-spin conversion in twisted graphene/WSe_2 heterostructures.
Lee SJ, de Sousa DJP, Kwon YK, de Juan F, Chi ZD, Casanova F, and Low T.
Physical Review B 106, 165420 (2022).

362 Structural and electronic properties of Na-B-H compounds at high pressure.
Li X, Zhang XH, Bergara A, Liu Y, and Yang GC.
Physical Review B 106, 174104 (2022).

363 Flat-band-induced superconductivity in synthetic bilayer optical lattices.
Salamon T, Irsigler B, Rakshit D, Lewenstein M, Grass T, and Chhajlany R.
Physical Review B 106, 174503 (2022).

364 Crystal structure and Raman-active lattice vibrations of magnetic topological insulators $MnBi_2Te_4{\cdot}n(Bi_2Te_3)$ (n=0, 1, ...,6).
Amiraslanov IR, Aliev ZS, Askerova PA, Alizade EH, Aliyeva YN, Abdullayev NA, Jahangirli ZA, Otrokov MM, Mamedov NT, and Chulkov EV.
Physical Review B 106, 184108 (2022).

365 Level occupation switching with density functional theory.
Sobrino N, Jacob D, and Kurth S.
Physical Review B 106, 195124 (2022).

366 Cavity-induced chiral edge currents and spontaneous magnetization in two-dimensional electron systems.
Sedov DD, Shirobokov V, Iorsh IV, and Tokatly IV.
Physical Review B 106, 205114 (2022).

367 Towards comprehension of the surface state properties in the intrinsic magnetic topological insulators.
Men'shov VN, Shvets IA, and Chulkov EV.
Physical Review B 106, 205301 (2022).

368 Transition from weak to strong light-molecule coupling: application to fullerene C_{60} multilayers in metallic cavity.
Despoja V, and Novko D.
Physical Review B 106, 205401 (2022).

369 Field-free anomalous junction and superconducting diode effect in spin-split superconductor/topological insulator junctions.
Kokkeler TH, Golubov AA, and Bergeret FS.
Physical Review B 106, 214504 (2022).

370 Absence of sizable superconductivity in hydrogen boride: a first-principles study.
Meninno A, and Errea I.
Physical Review B 106, 214508 (2022).

371 Electron correlations rule the phonon-driven instability in single-layer $TiSe_2$.
Novko D, Torbatian Z, and Loncaric I.
Physical Review B 106, 245108 (2022).

372 Electronic and magnetic properties of the topological semimetal $SmMg_2 Bi_2$.
Kundu AK, Pakhira S, Roy T, Yilmaz T, Tsujikawa M, Shirai M, Vescovo E, Johnston DC, Pasupathy AN, and Valla T.
Physical Review B 106, 245131 (2022).

373 Locality of spontaneous symmetry breaking and universal spacing distribution of topological defects formed across a phase transition.
del Campo A, Gomez-Ruiz FJ, and Zhang HQ.
Physical Review B 106, L140101 (2022).

374 Interaction-enhanced topological hall effects in strained twisted bilayer graphene.
Pantaleon PA, Phong VT, Naumis GG, and Guinea F.
Physical Review B 106, L161101 (2022).

375 Spin-orbit induced equilibrium spin currents in materials.
Droghetti A, Rungger I, Rubio A, and Tokatly IV.
Physical Review B105, 024409 (2022).

376 Dissipation and spontaneous emission in quantum electrodynamical density functional theory based on optimized effective potential: a proof of concept study.
Kudlis A, Iorsh I, and Tokatly IV.
Physical Review B105, 054317 (2022).

377 Measurement of the ^{136}Xe two-neutrino double-β-decay half-life via direct background subtraction in NEXT.
Novella P, Sorel M, Uson A, Adams C, Almazan H, Alvarez V, Aparicio B, Aranburu AI, Arazi L, and Arnquist IJ.
Physical Review C 105, 055501 (2022).

378 Cascading traffic jamming in a two-dimensional motter and Lai model.
Cwilich G, and Buldyrev SV.
Physical Review E 106, 024303 (2022).

379 Searching for hidden neutrons with a reactor neutrino experiment: constraints from the STEREO experiment.
Almazan H, Bernard L, Blanchet A, Bonhomme A, Buck C, Sanchez PD, El Atmani I, Labit L, Lamblin J, Letourneau A, et al.
Physical Review Letters 128, 061801 (2022).

380 Degradation of phonons in disordered moire superlattices.
Ochoa H, and Fernandes RM.
Physical Review Letters 128, 065901 (2022).

381 Joint measurement of the ^{235}U antineutrino spectrum by PROSPECT and STEREO.
Almazan H, Andriamirado M, Balantekin AB, Band HR, Bass CD, Bergeron DE, Bernard L, Blanchet A, Bonhomme A, Bowden NS, et al.
Physical Review Letters 128, 081802 (2022).

382 Superfluid weight bounds from symmetry and quantum geometry in flat bands.
Herzog-Arbeitman J, Peri V, Schindler F, Huber SD, and Bernevig BA.
Physical Review Letters 128, 087002 (2022).

383 Variational principle for optimal quantum controls in quantum metrology.
Yang J, Pang SS, Chen ZK, Jordan AN, and del Campo A.
Physical Review Letters 128, 160505 (2022).

384 Dynamics of two ferromagnetic insulators coupled by superconducting spin current.
Ojajarvi R, Bergeret FS, Silaev MA, and Heikkila TT.
Physical Review Letters 128, 167701 (2022).

385 Theory of the supercurrent diode effect in Rashba superconductors with arbitrary disorder.
Ilic S, and Bergeret FS.
Physical Review Letters 128, 177001 (2022).

386 Spin-polarizing electron beam splitter from crossed graphene nanoribbons.
Sanz S, Papior N, Giedke G, Sanchez-Portal D, Brandbyge M, and Frederiksen T.
Physical Review Letters 129, 037701 (2022).

387 Magic-angle twisted bilayer graphene as a topological heavy fermion problem.
Song Z, and Bernevig BA.
Physical Review Letters 129, 047601 (2022).

388 Reentrant correlated insulators in twisted bilayer graphene at 25 T (2π Flux).
Herzog-Arbeitman J, Aaron C, Dmitri E, and Bernevig A.
Physical Review Letters 129, 076401 (2022).

389 Unified approach to polarons and phonon-induced band structure renormalization.
Lafuente-Bartolome J, Lian C, Sio WH, Gurtubay IG, Eiguren A, and Giustino F.
Physical Review Letters 129, 076402 (2022).

390 Spectroscopy of twisted bilayer graphene correlated insulators.
Calugaru D, Regnault N, Oh M, Kevin P, Nuckolls JP, Wong D, Lee RL, Yazdani A, Vafek O, and Bernevig BA.
Physical Review Letters 129, 117602 (2022).

391 Skyrmion echo in a system of interacting skyrmions.
Wang XG, Guo GH, Dyrdal A, Barnas J, Dugaev VK, Parkin SSP, Ernst A, and Chotorlishvili L.
Physical Review Letters 129, 126101 (2022).

392 One-dimensional quantum systems withg ground state of jastrow form are integrable.
Yang J, and del Campo A.
Physical Review Letters 129, 150601 (2022).

393 Dramatic plasmon response to the charge-density-wave gap development in 1T-$TiSe_2$.
Lin ZJ, Wang CX, Balassis A, Echeverry JP, Vasenko AS, Silkin VM, Chulkov EV, Shi YG,
Zhang JD, Guo JD, and Zhu XT.
Physical Review Letters 129, 187601 2022).

394 Probing the role of grain boundaries in single Cu nanoparticle oxidation
by in situ plasmonic scattering.
Nilsson S, Posada-Borbon A, Zapata-Herrera M, Fanta ABD, Albinsson D, Fritzsche J, Silkin VM, Aizpurua J,
Gronbeck H, Esteban R, and Langhammer C.
Physical Review Materials 6, 045201 (2022).

395 Photon tunneling reconstitution in black phosphorus/hBN heterostructure.
Zhou CL, Zhang Y, Torbatian Z, Novko D, Antezza M, and Yi HL.
Physical Review Materials 6, 075201 (2022).

396 Electronic structure of antiferromagnetic Dirac semimetal candidate $GdIn_3$.
Yin ZX, Du X, Zhang S, Chen C, Pei D, Zhou JS, Gu X, Xu RZ, Zhang QQ, Zhao WX, et al.
Physical Review Materials 6, 084203 (2022).

397 Dynamic portfolio optimization with real datasets using quantum processors
and quantum-inspired tensor networks.
Mugel S, Kuchkovsky C, Sanchez E, Fernandez-Lorenzo S, Luis-Hita J, Lizaso E, and Orus R.
Physical Review Research 4, 013006 (2022).

398 Uncertainty relations with the variance and the quantum Fisher information
based on convex decompositions of density matrices.
Toth G and Frowis F.
Physical Review Research 4, 013075 (2022).

399 Super-Heisenberg scaling in Hamiltonian parameter estimation in the long-range Kitaev chain.
Yang J, Pang SS, del Campo A, and Jordan AN.
Physical Review Research 4, 013133 (2022).

400 Digitized-counterdiabatic quantum approximate optimization algorithm.
Chandarana P, Hegade NN, Paul K, Albarran-Arriagada F, Solano E, del Campo A, and Chen X.
Physical Review Research 4, 013141 (2022).

401 Effect of the valence state on the band magnetocrystalline anisotropy
in two-dimensional rare-earth/noble-metal compounds.
Blanco-Rey M, Castrillo-Bodero R, Ali K, Gargiani P, Bertran F, Sheverdyaeva PM, Ortega JE,
Fernandez L, and Schiller F.
Physical Review Research 4, 013237 (2022).

402 Benchmarking quantum annealing dynamics: The spin-vector Langevin model.
Subires D, Gomez-Ruiz FJ, Ruiz-Garcia A, Alonso D, and del Campo A.
Physical Review Research 4, 023104 (2022).

403 Theory of longitudinal and transverse nonlinear dc conductivity.
Resta R.
Physical Review Research 4, 033002 (2022).

404 Long-range electron-electron interactions in quantum dot systems and applications
in quantum chemistry.
Knorzer J, van Diepen CJ, Hsiao TK, Giedke G, Mukhopadhyay U, Reichl C, Wegscheider W,
Cirac JI, and Vandersypen LMK.
Physical Review Research 4, 033043 (2022).

405 Probing quantum chaos in multipartite systems.
Cao Z, Xu ZY, and del Campo A.
Physical Review Research 4, 033093 (2022).

406 Relaxation of photoexcited hot carriers beyond multitemperature models:
General theory description verified by experiments on Pb/Si(111).
Kratzer P, Rettig L, Sklyadneva IY, Chulkov EV, and Bovensiepen U.
Physical Review Research 4, 033218 (2022).

407 Ab initio electronic stationary states for nuclear projectiles in solids.
Halliday JFK, Famili M, Forcellini N, and Artacho E.
Physical Review Research 4, 043077 (2022).

408 Moire dispersion of edge states in spin chains on superconductors.
Mier C, Choi DJ, and Lorente N.
Physical Review Research 4, L032010 (2022).

409 Topological order in random interacting Ising-Majorana chains stabilized by many-body localization.
Laflorencie N, Lemarie G, and Mace N.
Physical Review Research 4, L032016 (2022).

410 Mapping lamb, stark, and purcell effects at a chromophore-picocavity junction with hyper-resolved fluorescence microscopy.
de Roslawska A, Neuman T, Doppagne B, Borisov AG, Romeo M, Scheurer F, Aizpurua J, and Schull G.
Physical Review X 12, 011012 (2022).

411 Unifying quantum and classical speed limits on observables.
Garcia-Pintos LP, Nicholson SB, Green JR, del Campo A, and Gorshkov AV.
Physical Review X 12, 011038 (2022).

412 Neutral bremsstrahlung emission in xenon unveiled.
Henriques CAO, Amedo P, Teixeira JMR, Gonzalez-Diaz D, Azevedo CDR, Para A, Martin-Albo J, Hernandez AS, Gomez-Cadenas JJ, Nygren DR, et al.
Physical Review X 12, 021005 (2022).

413 Gamma gamma decay as a probe of neutrinoless ββ decay nuclear matrix elements.
Romeo B, Menendez J, and Garay CP.
Physics Letters B 827, 136965 (2022).

414 Bio-based semi-crystalline PEF: temperature dependence of the constrained amorphous interphase and amorphous chain mobility in relation to crystallization.
Righetti MC, Vannini M, Celli A, Cangialosi D, and Marega C.
Polymer 247, 124771 (2022).

415 Comment on "Anomalous structural recovery in the near glass transition range in a polymer glass: data revisited in light of temperature variability in vacuum oven-based experiments".
Cangialosi D, Alegria A, and Colmenero J.
Polymer Engineering and Science 62, 2716 (2022).

416 Approaching polymer dynamics combining artificial neural networks and elastically collective nonlinear Langevin equation.
Miccio LA, Borredon C, Casado U, Phan AD, and Schwartz GA.
Polymers 14, 1573 (2022).

417 Self-healing and reprocessable oleic acid-based elastomer with dynamic S-S bonds as solvent-free reusable adhesive on Copper surface.
Pettazzoni L, Leonelli F, Marrani AG, Migneco LM, Vetica F, Celio L, Napoleone V, Alfano S, Colecchia A, Amato F, et al.
Polymers 14, 4919 (2022).

418 Macrocyclic polymers: synthesis, purification, properties and applications.
Ochs J, Pagnacco CA, and Barroso-Bujans F.
Progress in Polymer Science 134, 101606 (2022).

419 Properties and challenges of hot-phonon physics in metals: MgB_2 and other compounds.
Cappelluti E, Caruso F, and Novko D.
Progress in Surface Science 97, 100664 (2022).

420 Review of particle physics.
Workman RL, Burkert VD, Crede V, Klempt E, Thoma U, Tiator L, Agashe K, Aielli G, Allanach BC, Amsler C, et al.
Progress of Theoretical and Experimental Physics 2022, 083C01 (2022).

421 Quantum speed limits on operator flows and correlation functions.
Carabba N, Hornedal N, and del Campo A.
Quantum 6, 884 (2022).

422 Bragg's additivity rule and core and bond model studied by real-time TDDFT electronic stopping simulations: the case of water vapor.
Gu B, Munoz-Santiburcio D, Cleri F, Artacho E, Kohanoff J, and Da Piev F.
Radiation Physcis and Chemistry 193, 109961 (2022).

423 Quantum many-body scars and Hilbert space fragmentation: a review of exact results.
Moudgalya S, Bernevig BA, and Regnault N.
Reports on Progress in Physics 85, 086501 (2022).

424 Spoof surface plasmon photonics.
Garcia-Vidal FJ, Fernandez-Dominguez AI, Martin-Moreno L, Zhang HC, Tang WX, Peng RW, and Cui TJ.
Reviews of Modern Physics 94, 025004 (2022).

425 Engineering quantum states and electronic landscapes through surface molecular nanoarchitectures.
Piquero-Zulaica I, Lobo-Checa J, Abd El-Fattah ZM, Ortega JE, Klappenberger F, Auwarter W, and Barth JV.
Reviews of Modern Physics 94, 045008 (2022).

426 Inelastic scattering of electrons in water from first principles: cross sections and inelastic mean free path for use in Monte Carlo track-structure simulations of biological damage.
Koval NE, Koval P, Da Pieve F, Kohanoff J, Artacho E, and Emfietzoglou D.
Royal Society Open Science 9, 212011 (2022).

427 Ultrahard magnetism from mixed-valence dilanthanide complexes with metal-metal bonding.
Gould CA, McClain KR, Reta D, Kragskow JGC, Marchiori DA, Lachman E, Choi ES, Analytis JG, Britt RD, Chilton NF, et al.
Science 375, 198 (2022).

428 All topological bands of all nonmagnetic stoichiometric materials.
Vergniory MG, Wieder BJ, Elcoro L, Parkin SSP, Felser C, Bernevig BA, and Regnault N.
Science 376, 816 (2022).

429 Negative reflection of nanoscale-confined polaritons in a low-loss natural medium.
Alvarez-Perez G, Duan JH, Taboada-Gutierrez J, Ou QD, Nikulina E, Liu S, Edgar JH, Bao QL, Giannini V, Hillenbrand R, et al.
Science Advances 8, eabp8486 (2022).

430 Bacterial biofilms on medical masks disposed in the marine environment: a hotspot of biological and functional diversity.
Crisafi F, Smedile F, Yakimov MM, Aulenta F, Fazi S, La Cono V, Martinelli A, Di Lisio V, and Denaro R.
Science of the Total Environment 837, 155731 (2022).

431 Tailoring magnetism in silicon-doped zigzag graphene edges.
Ugartemendia A, Garcia-Lekue A, and Jimenez-Izal E.
Scientific Reports 12, 13032 (2022).

432 Electron microscopy and calorimetry of proteins in supercooled water.
Melillo JH, Nikulina E, Iriarte-Alonso MA, Cerveny S, and Bittner AM.
Scientific Reports 12, 16512 (2022).

433 Localization versus delocalization of d-states within the Ni_2MnGa Heusler alloy.
Janovec J, Zeleny M, Heczko O, and Ayuela A.
Scientific Reports 12, 20577 (2022).

434 Manifold curvature and Ehrenfest forces with a moving basis.
Halliday JFK, and Artacho E.
Scipost Physics 12, 020 (2022).

435 Assessing the role of interatomic position matrix elements in tight-binding calculations of optical properties.
Ibanez-Ibanez J, de Juan F, and Souza I.
Scipost Physics 12, 070 (2022).

436 Fingerprints of hot-phonon physics in time-resolved correlated quantum lattice dynamics.
Cappelluti E, and Novko D.
Scipost Physics 12, 173 (2022).

437 Landau levels in curved space realized in strained graphene.
Wagner G, de Juan F, and Nguyen DX.
Scipost Physics Core 5, 029 (2022).

438 Data compression in the NEXT-100 data acquisition system.
Bosch RE, Ponce JR, Estevez AS, Rodriguez JMB, Bosch VH, and Alarcon JFT.
Sensors 22, 5197 (2022).

439 A comparative analysis of human behavior prediction approaches in intelligent environments.
Almeida A, Bermejo U, Bilbao A, Azkune G, Aguilera U, Emaldi M, Dornaika F, and Arganda-Carreras I.
Sensors 22, 701 (2022).

440 Study of an energy-harvesting damper based on magnetic interaction.
Aberturas S, Hernando A, Olazagoitia JL, and Garcia MA.
Sensors 22, 7865 (2022).

441 X-ray photon correlation spectroscopy towards measuring nanoparticle diameters in biological environments allowing for the in situ analysis of their bio-nano interface.
Otto F, Sun X, Schulz F, Sanchez-Cano C, Feliu N, Westermeier F, and Parak WJ.
Small 18, 2201324 (2022).

442 Probing the effect of rigidity on the cellular uptake of core-shell nanoparticles: stiffness effects are size dependent.
Gurnani P, Sanchez-Cano C, Xandri-Monje H, Zhang JL, Ellacott SH, Mansfield EDH, Hartlieb M, Dallmann R, and Perrier S.
Small 18, 2203070 (2022).

443 Physical aging of hydroxypropyl methylcellulose acetate succinate via enthalpy recovery.
Seo Y, Zuo B, Cangialosi D, and Priestley RD.
Soft Matter 18, 8331 (2022).

444 Atom scattering as a probe of the surface electron-phonon interaction at conducting surfaces.
Manson JR, Benedek G, and Miret-Artes A.
Surface Science Reports 77, 100552 (2022).

445 Structural instability at the in-terminated surface of the heavy-fermion superconductor $CeIrIn_5$.
Tarasov AV, Mende M, Ali K, Poelchen G, Schulz S, Vilkov OY, Bokai KA, Muntwiler M, Mandic V, Laubschat C, et al.
Surfaces and Interfaces 32, 102126 (2022).

446 Geopolymer concrete performance study for high-temperature thermal energy storage (TES) applications.
Rahjoo M, Goracci G, Martauz P, Rojas E, and Dolado JS.
Sustainability 14, 1937 (2022).

447 Induced vacuum energy density of quantum charged scalar matter in the background of an impenetrable magnetic tube with the neumann boundary condition.
Gorkavenko VM, Gorkavenko TV, Sitenko YA, and Tsarenkova MS.
Ukranian Journal of Physics 67, 715 (2022).

448 Radon mitigation applications at the laboratorio subterraneo de Canfranc (LSC).
Perez-Perez J, Amare JC, Bandac IC, Bayo A, Borjabad-Sanchez S, Calvo-Mozota JM, Cid-Barrio L, Hernandez-Antolin R, Hernandez-Molinero B, and Novella P.
Universe 8, 112 (2022).

449 Restricted active space configuration interaction methods for strong correlation: recent developments.
Casanova D.
Wiley Interdisciplinary Reviews Computational Molecular Science 12, e1561 (2022).

450 Transport and optical properties of the chiral semiconductor Ag_3AuSe_2.
Won J, Kim S, Gutierrez-Amigo M, Bettler S, Lee B, Son J, Noh TW, Errea I, Vergniory MG, Abbamonte P, et al.
Zeitschrift fur Anorganische und Allgemeine Chemie 648, 202200055 (2022).

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Pictured here is the DIPC Community
outside the headquarters in Donostia/San Sebastián.

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Jesus M. Ugalde UPV/EHU
Lucia Vitali UPV/EHU
Nerea Zabala UPV/EHU

Ikerbasque Research Professors

Slawomir Grabowski
01/01/2012–Present
Hydrogen bonds in gas phase and crystals; quantum theory of atoms in molecules and natural bond orbitals approaches; intermolecular interactions as preliminary stages of chemical reactions.

Andreas Heidenreich
01/01/2012–Present
Computer simulations of nanoplasma formation, Coulom explosions and nuclear fusion induced by ultraintense and ultrashort laser pulses. Computer simulations of pump-probe signals.

Eugene Krasovskii
01/01/2012–Present
Electronic structure of surfaces and interfaces and computational spectroscopy: electron diffraction, angle and time-resolved photoemission, and dielectric response from first principles.

Mario Piris Silvera
01/01/2012–Present
Energy functional method development. Computational modelling of semiconductor nanocluster and molecular solid phases and polymorfism.

Vyacheslav Silkin
01/01/2012–Present
Ultrafast dynamics of the one-particle and collective electronic excitations in metals and their surfaces. The study of electronic excitations at adsorbates on metal surfaces.

Thomas Frederiksen
15/08/2012–Present
Nanoelectronics - theory and simulation.

Geza Giedke
01/09/2014–Present
Quantum systems and technologies.

Fabienne Barroso Bujans
01/02/2016–Present
Novel complex-shaped cyclic polymers, from synthesis to plysical properties. Devices and nanodevices based on cyclic polymers/graphene hybrid materials.

Luca Salassa
01/01/2017–Present
Development of photoactivatable anticancer metal complexes and nanomaterials. Experimental and computational inorganic photochemistry.

Denis Vyalykh
01/01/2017–Present
Photoemission measurements of magnetic surface states.

Juan José Gómez Cadenas
14/03/2018–Present
Experimental particle physics.

Román Orús Lacort
01/09/2018–Present
Quantum systems and technologies.

Francisco Guinea López
01/09/2019–01/09/2022
Two dimensional materials.

Miguel Ángel Cazalilla Gutiérrez
01/09/2020–Present
Investigation of the load and spin transport properties in low dimensional systems, highly correlated systems and superconductors. Quantum dissipation and non-balance effects.

Nathan John Bastian
01/03/2021–Present
Stellar population studies.

Juan Ignacio Collar Colmenero
23/11/2022–Present
Neutrino physics at the European Spallation Source.

Distinguished Researchers

Irina Sklyadneva
01/05/2003–Present
Electron-phonon coupling in the 3D topological isolators and Weil semiconductors as well as and in ultrathin lead and indium films on the Si substrate (superconductivity).

Albert Fert
01/01/2020–Present
Conversion between spin and charge currents at room temperature by Rashba or topological insulator interfaces, 2D magnets and perspective for low power spintronic devices.

George Fitzgerald Smoot
01/11/2020–Present
Measuring the sum of neutrino masses and properties, interpreting LIGO/Virgo events and testing the nature of Dark Matter.

Cheol Hwan Park
01/03/2022–Present
Topological, anomalous, and spin-Hall conductivities from effective field theory and first-principles calculations.

Roman Kuzian
01/07/2022–Present
Time-resolved photoemission from solids.

Anatolii V. Goncharenko
01/09/2022–Present
Plasmonics and nanooptics.

Francisco Guinea López
01/09/2022–Present
Two dimensional materials.

Tonica Valla
01/10/2022–Present
Condensed Matter Physics – Emergent Phenomena at Quantum Interfaces.

Ikerbasque Research Associates

Aran García-Lekue
01/11/2017–Present
Modeling electron transport at the nanoscale. Theoretical investigation of electron processes at nanostructured surface.

Paola Ferrario
01/12/2017–Present
Naeutrino physics.

Alexey Nikitin
01/01/2018–Present
Nanophotonics of 2D materials.

Miguel Moreno Ugeda
01/04/2018–Present
Low-temperature scanning tunneling microscopy and spectroscopy of two-dimensional materials and nanostructures.

Raúl Esteban Angulo de la Fuente
01/06/2018–Present
Numerical simulations in cosmology.

David Casanova Casas
01/07/2018–Present
Electronic structure of molecular excited states and photophysical process: theory and applications.

Dario Bercioux
01/10/2019–Present
Quantum transport in nanostructures.

Santiago Blanco Canosa
01/10/2019–Present
Synchrotron research in high Tc superconductors and low dimensional ferromagnets.

Eduard Matito Gras
15/03/2020–Present
Development of electronic structure methods and real-space descriptors of chemical bonding and aromaticity.

Iván Rivilla De la Cruz
01/02/2021–Present
Field of molecular indicators for single atom detection in dry media, with major applications to neutrino physics and a clear potential for biomedical.

Francesc Monrabal Capilla
01/02/2022–Present
Development of xenon detectors for basic and applied physics.

Fellows

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

Maia García Vergniory
01/05/2021–Present
Prediction of new topological phases and materials.

Ikerbasque Research Fellows

Silvia Bonoli
01/09/2018–Present
Formation and evolution of supermassive black holes in a cosmological context, combining theoretical models and observational data.

Fernando De Juan Sanz
01/09/2018–Present
Topology and electronic correlations in quantum materials.

Francesc Monrabal Capilla
01/07/2019–31/01/2022
Development of xenon detectors for basic and applied physics.

Aitzol García Etxarri
01/11/2019–Present
Nanophotonics theory.

Bo Chen
18/02/2020–Present
Nanothread chemistry and physics; high-pressure chemistry; carbene and diradical chemistry.

Carlos Sánchez Cano
01/09/2021–Present
Controlling the metabolism of cells using metal-based intracellular catalysts.

Héctor Ochoa De Eguileor
01/11/2021–31/12/2022
Electronic correlations in two-dimensional materials.

Tobias Daniel Grass
01/10/2022–Present
Quantum simulation and synthetic quantum matter.

Postdoctoral Positions

Abel Carreras Conill
01/04/2018–Present
Development of electronic structure methods for excited states.

Matteo Zennaro
01/07/2018–28/09/2022
Cosmological structure formation.

Marcos Pellejero Ibáñez
01/10/2018–Present
Cosmological N-body simulations and the analysis of the large-scale structure of the universe.

Marcelo José Ambrosio
25/03/2019–24/03/2022
Theoretical description of photoemission processes at the attosecond scale.

Wan Wen
11/04/2019–Present
Growth and characterization of 2D materials and related heterostructures.

Fernando Javier Gómez Ruiz
22/07/2019–31/01/2022
Tailoring quantum matter far away from equilibrium.

Jens Oliver Stücker
02/09/2019–Present
Cosmology.

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

Fernando Aguilar-Galindo Rodríguez
15/01/2020–09/01/2022
Quantum chemistry calculations of molecules adsorbed on surfaces for applications in nanophotonics including ultra-fast spectroscopy and surface-enhanced spectroscopy.

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

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

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

Mikel Odriozola Gimeno
01/08/2020–31/08/2022
Synthesis of fluorophores for detection of SARS-Cov 2.

Julio Jonás Chaves Montero
01/10/2020–16/09/2022
Astrophysics and cosmology.

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

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

José María Benlloch Rodríguez
22/01/2021–21/01/2022
Development of an image reconstruction software for a full-body PET based on liquid xenon.

Uxua Huici Rayo
25/01/2021–31/03/2022
Design, synthesis and characterization of lanthanide based chiral and enantiopure MOFs for CISS effect studies.

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

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

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

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

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

Mihovil Bosnar
01/10/2021–09/05/2022
Condensed matter physics.

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

Ana Cristina Carrasco Gento
12/10/2021–31/12/2022
Biorthogonal photocatalysis towards metal substrates.

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

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

Rodrigo Voivodic
06/12/2021–31/12/2022
Cosmology–Large scale structure.

Nahual Carlos Sobrino Coll
16/12/2021–31/07/2022
Electronic and thermal transport through strongly correlated system
as described by density functional theory.

Mikel Irigoyen Urtasun
01/01–31/12/2022
Theoretical simulations of the gold-PTEBS interface for artificial photosynthesis.

Rodrigo Ezequiel Menchón Turco
01/01–31/12/2022
Computational design of spin-quantum systems in graphene nanostructures.

Jorge Olmos Trigo
01/01–30/09/2022
Chiral optomechanical interactions.

José Luis Montaño Priede
19/01/2022–Present
Computational electrodynamics for light control in plasmonic systems.

Iñigo Robredo Magro
01/02/2022–Present
Topological quantum materials as platforms for quantum computers.

Jorge Humberto Melillo
07/02/2022–Present
Supercooled water–polymeric and biological aqueous solutions.

Roberto Álvarez Boto
01/03/2022–Present
Quantum Technologies–Optical properties of doped nanographenes.

María Blanco De Paz
01/03/2022–Present
Quantum Technologies–Quantum metasurfaces.

Beatriz Robles Hernández
01/03/2022–Present
Polymers and soft matter.

Ander Simón Estévez
01/03/2022–Present
Coherent neutrino-nucleus scattering at ESS.

Alexey Brodoline
08/03/2022–Present
Optics, fluorescence.

Camillo Tassi
28/03/2022–Present
Quantum technologies: quantum simulation in condensed-matter and ultracold atom platforms.

Luis Alejandro Miccio Stefancik
01/04/2022–Present
Chain dynamics in crosslinked filled polymer systems with high plasticizer content.

María Isabel Ardaya Franco
04/04/2022–Present
Neurobioscience–nanoneuro: optically manipulating neuronal activity with nanoparticles.

Miguel Ángel Sánchez Martínez
09/05/2022–Present
Chiral superconductors in transition metal dichalcogenides.

Eloy Ramos Córdoba
01/06/2022–Present
Benchmarking of density functional approximations.

Juan Carlos Roldao
23/06/2022–Present
Theoretical treatment of optoelectronic properties and processes of organic compounds
for energy and material conversion.

Ridwan Olamide Agbaoye
27/06/2022–Present
Ab-initio description of thermodielectric properties of zeolites and cement-based materials.

Anastasiia Skurativska
11/07/2022–Present
Quantum Technologies–Quantum annealing hardwarebased on non-conventional superconducting circuitsand new quantum materials.

Nicodemos Varnava
03/08–03/10/2022
Theoretical Condensed Matter Physics.

Haoyu Hu
22/09/2022–Present
Development of flat band theory methods for search of new materials.

Roberto Stefano Soleti
26/09/2022–Present
Neutrinoless double-beta decay with the NEXT experiment.

Raphael Enoque De Paiva
30/09/2022–Present
Development of photoactivatable anticancer metal complexes and nanomaterials.

Sofía Sanz Wuhl
22/10/2022–Present
Theory of quantum transport in graphene-based nanostructure networks.

Siddhartha Patra
18/11/2022–Present
Tensor Networks and Artificial Intelligence for Quantum Matter.

Douglas Nakahata
21/11/2022–Present
Metal catalysis for the chemical modification of proteins.

Mario Fernández Pendás
01/12/2022–Present
Molecular simulations of protein aggregation.

Carmelo Naim
19/12/2022–Present
Computational chemistry.

Research Collaborators

Ilya Nechaev
01/11/2020–16/01/2022
Linear response, low-energy electron scattering, and photoemission within the relativistic k.p methodology.

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

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

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

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

Amjad Al Taleb
01/03/2022–Present
Study of surface catalysis using molecular beams.

PhD Students

Paul Dreher
08/01/2018–07/01/2022
Manipulation of collective ground states in highly correlated transition meal dichalcogenides.

Xiang Xu
21/02/2018–20/02/2022
Study of intraocular functions.

José Manuel Lanuza Delgado
01/03/2018–28/02/2022
QM and QM/MM simulations of phosphate drydrolysis reactions catalized in various environments.

Joscha Kruse
01/04/2018–29/03/2022
Dynamic self-assembly of plasmonic nanoparticles in flow.

Masoud Mansouri
20/05/2018–20/05/2022
Electronic excitations in organ metallic compounds.

Irene Ruiz Ortiz
01/09/2018–31/08/2022
Intrinsically disordered drug discovery.

Unai Muniain Caballero
01/10/2018–30/09/2022
Classical and ab-initio study of optical surface excitations for nanophotonics.

Auguste Tetenoire
01/10/2018–30/09/2022
Molecular dynamics simulations of femtosecond laser induced desorption of adsorbates from metal surfaces.

Alejandro Berdonces Layunta
22/10/2018–21/10/2022
Functional materials synthesized by surface-supported chemistry under vacuum.

Sophie Espert
01/11/2018–31/10/2022
Protonic conductivity mechanism in new electrolytes based on strong acid clathrate hydrates.

María Zubiría Ulacia
01/11/2018–31/10/2022
Triplet states in PDI and related organic molecules.

Álvaro Pozo Larrocha
08/11/2018–08/11/2022
Axionic wave dark matter project.

Pablo Herrero Gómez
01/01/2019–31/12/2022
Development of hardware an analysis for SABBAT project.

Ricardo Rama Eiroa
03/12/2019–02/01/2022
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
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 and 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.

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

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

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

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

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

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

Francesco Gambino
01/09/2021–31/08/2022
Photocatalysis towards metal substrates and its applications.

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

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

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

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

Markos Polkas
15/10/2021–Present
Supermassive black holes and galaxy evolution.

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

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

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

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

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

Sara Ortega Martínez
01/01/2022–Present
Cosmos: computational cosmology.

David Silva Brea
01/01/2022–Present
Theoretical simulations on the interaction of metals with intrinsically disordered peptide.

Duy Hoang Minh Nguyen
12/01/2022–Present
Twisted 2D materials.

Andrei Paulau
12/01/2022–Present
Theoretical chemistry.

Leire Larizgoitia Arcocha
17/01/2022–Present
Development of gaseous detectors for the ESS.

Javier Antonio Vélez Simanca
31/01/2022–Present
3D ferromagnetic and antiferromagnetic texture dynamics in curved geometries.

Tim Kokkeler
07/02/2022–Present
Transport properties of non-conventional superconducting structures.

Amitayush Jha Thakur
11/04/2022–Present
Condensed matter physics.

Chen-How Huang
03/05/2022–Present
Low dimensional system, quantum systems in non-equilibrium.

Andrés Felipe Bejarano Sánchez
06/05/2022–Present
Quantum transport.

Nino Lauber
09/05/2022–Present
Origins/emergence of metabolism.

Julen Aduriz Arrizabalaga
13/05/2022–Present
Theoretical simulation of metal-Abeta complexes.

Teresa Itziar Celaya Garmendia
17/05/2022–Present
Nanoneuro: optically manipulating neuronal activity with nanoparticles.

Helene Müller
30/06/2022–Present
Electronic properties at the nanoscale.

Nerea Salor Iguíñiz
01/08/2022–Present
Medical Physics.

Jinxiu Zhou
08/08/2022–Present
Helix polymer based on unnatural densely substitute propeline.

Nils Hoyer
01/09/2022–Present
The cosmological evolution of Nuclear Star Clusters.

Sandra Sajan
01/09/2022–Present
Unconventional superconductivity in 2D materials.

María De los Ángeles Del Barrio Torregrosa
01/10/2022–Present
Neutrinoless double beta decay with the NEXT experiment.

Eric Gómez Urreizti
01/10/2022–Present
Synthesis of cyclic polymers for biomedical applications.

Josianne Imbola Owona
01/10/2022–Present
Theoretical Chemistry and Computational Modelling

Antonio Morales Pérez
01/10/2022–Present
Artificial Intelligence algorithms for the topological control of quantum emitters.

Carmelo Naim
01/11–18/12/2022
Computational chemistry.

Marc Montilla Busquets
21/11/2022–Present
Nonlinear optical properties, decomposition, origin-independence.

Pablo Bermejo Navas
01/12/2022–Present
Hybrid quantum machine learning for NISQ devices. Analysis of QML methods, tensor networks and neuromorphic computing.

Marta Costa Verdugo
15/12/2022–Present
Development of new photocatalytic materials for drug delivery.

Javier Domínguez Calvo
19/12/2022–Present
Development of new density functional approximations.

Research Assistants

Augustin Mathias
27/01/2021–16/05/2022

María Blanco De Paz
27/03/2021–27/01/2022

Andrés Felipe Bejarano Sánchez
06/05/2021–05/05/2022

Teresa Itziar Celaya Garmendia
17/05/2021–16/05/2022

Leire Larizgoitia Arcocha
01/09/2021–16/01/2022

Mikel Olano Aramburu
01/09/2021–Present

Sofía Sanz Wuhl
07/09/2021–21/10/2022

Ebtisam Tarek Mohammed Saeed
15/10/2021–Present

Raúl Guerrero Avilés
27/10/2021–31/12/2022

Haritz Garai Marín
15/11/2021–31/12/2022

Iñigo Robredo Magro
16/11/2021–31/01/2022

Pablo Bermejo Navas
01/12/2021–30/11/2022

Joaquín Sureda Hernández
13/12/2021–31/10/2022

Marta Costa Verdugo
15/12/2021–14/12/2022

Javier Domínguez Calvo
01/01–18/12/2022

Maialen Galdeano Fraile
01/01/2022–Present

Paul Dreher
08/01–30/03/2022

Sandra Sajan
07/02–31/08/2022

Xiang Xu
21/02–20/08/2022

Joscha Kruse
30/03–31/07/2022

Ane Izaskun Aranburu Leiva
09/05/2022–Present

Masoud Mansouri
21/05–01/12/2022

Carlos Alberto Maciel Escudero
01/07/2022–Present

Cristina Mier González
01/09/2022–Present

Mikel Elorza Romera
14/09/2022–Present

Martin Irízar Landa
01/10/2022–Present

Alaitz Lecuona Isasa
01/10/2022–Present

Paloma Morilla Martínez
01/10/2022–Present

Unai Muniain Caballero
01/10/2022–Present

Auguste Tetenoire
01/10/2022–Present

Ainhoa Villoria Bárcena
01/10/2022–Present

Mireia Tena Zuazolacigorraga
12/10/2022–31/12/2022

Carolina Martínez Strasser
13/10/2022–Present

Miguel Ángel Jiménez Herrera
17/10/2022–Present

Jon Lasa Alonso
17/10/2022–Present

Alejandro Berdonces Layunta
22/10/2022–Present

Sophie Espert
01/11/2022–Present

Álvaro Pozo Larrocha
09/11/2022–Present

Riccardo Moro
21/11/2022–Present

Mikel Iraola Iñurrieta
22/11/2022–Present

Daniel García Pina
28/11/2022–Present

Álvaro Nodar Villa
01/12/2022–Present

Engineers

Jordi Torrent Collell
16/06/2018–Present

Eva Oblak
14/09/2020–Present

Rubén González Moreno
21/09/2020–31/01/2022

Ana Belén Núñez Chico
25/01/2021–Present

José María Benlloch Rodríguez
22/01/2022–Present

Sergio Sánchez Martín
01/02/2022–Present

Asier Castillo Litago
02/02/2022–Present

Alejandro Taboada Fernández
11/03/2022–Present

Technical Assistants

Beatriz Romeo Zaragozano
01/11/2018–Present

José Luis López Gómez
15/09/2020–02/10/2022

Francisco López Gejo
01/01/2021–Present

Edurne Sáenz Párraga
25/10/2021–24/10/2022

Carlos Echeverría Lizarraga
01/03/2022–Present

Bruno López-Gómez Saldaña
11/03/2022–Present

Jon Zapata Muñoz
01/12/2022–Present

Internships

Daniel Ruskov
UPV/EHU, Spain
01/12/2021–28/02/2022
Informatics Engineering.

Julen Galarza Burguete
UPV/EHU, Spain
03/01–31/03/2022
Analysis and improvement of the execution processes of scientific applications in DIPC supercomputing systems.

Unai Salas Lavesa
UPV/EHU, Spain
21/02–13/02/2022
Analysis and improvement of the execution processes of scientific applications in DIPC supercomputing systems.

Eduard Florin
IES Zubiri Manteo, Spain
02/03–02/06/2022
Technical engineer in telecommunications and IT systems.

Josianne Imbola Owona
University of Hamburg, Germany
01/05–31/07/2022
Chemistry.

Marta Apezteguía
UPV/EHU, Spain
24/05–23/07/2022
Reactivity and stability of N-centered radicals.

June Aguirre Tolosa
UPV/EHU, Spain
01/06–31/07/2022
Cyclic poly (ethylene glycol) as nanoparticle surface ligand: physisorption vs chemisorption.

Pablo Ramón García Valle
UPV/EHU, Spain
01/06–31/07/2022
Luminescent organometallic complexes: synthesis and functionalization of surfaces.

Iván Hidalgo Cenalmor
UPV/EHU, Spain
01/06–31/07/2022, 01/12/2022–Present
Biomedical Computer Vision: deep learning based super-resolution.

Mikel Loizate Gutiérrez-Cañas
Universidad de Oviedo, Spain
01/06–26/07/2022
Computational study of cyclopentadienone iron complexes.

Antonio Morales Pérez
UPV/EHU, Spain
01/06–31/07/2022
Fermi arcs in chiral photonics crystals.

Xuban Gastearena Irigoyen
UPV/EHU, Spain
02/06–01/08/2022
Theoretical characterization of the reaction mechanism to synthesize cyclic and linear polyethers.

Manuel Pérez Escribano
Katholieke Universiteit Leuven, Belgium
13/06–12/08/2022
Tuning the diradical character of organic molecules by rational design.

Ania Beatriz Rodríguez Barrera
Universidad Autónoma de Madrid, Spain
13/06–12/08/2022
Computational study of the effect of pressure on the thermal dimerization of cycloheptatriene.

Pablo Blanco Mas
Universidad Complutense de Madrid, Spain
15/06–31/08/2022
Particle physics.

Adelina López Romera
Universidad de Murcia, Spain
15/06–31/07/2022
Manufacturing nanodevices with atomic precision.

Pablo García Aragoneses
Imperial College, United Kingdom
20/06–20/08/2022
Angle resolved photoemission in 2D materials.

Borja Moralejo Tobajas
UPV/EHU, Spain
27/06–27/08, 26/09–06/11/2022
Analysis and improvement of the execution processes of scientific applications in DIPC supercomputing systems.

Marlene Bósquez Fuentes
Universidad de Valencia, Spain
01/07–31/08/2022
Molecular dynamics study of calmodulin in potassium channels.

Itziar Campo Juarros
Universidad de Valladolid, Spain
01/07–31/08/2022
Molecular dynamics study of calmodulin in potassium channels.

Dobromila Danková
Pavol Jozef Safarik University in Kosice, Slovakia
01/07–31/08/2022
Aromaticity and magnetic properties in large conjugated rings.

María Jiménez Puyuelo
Universidad de Zaragoza, Spain
01/07–15/09/2022
Particle physics.

Jon Moriñigo Mazo
UPV/EHU, Spain
01/07–31/08/2022
Analysis and improvement of the execution processes of scientific applications
in DIPC supercomputing systems.

Hamidur Rahman
Universidad de Valencia, Spain
01/07–31/08/2022
Design of bright unpaired electrons for optoelectronics.

Alejandro Ramos Alonso
Universidad Complutense de Madrid, Spain
01/07–31/08/2022
Soft modes of moiré patterns.

Gema Raposo Hernández
Universidad de Oviedo, Spain
01/07–31/07/2022
Conformational entropy of intrinsically disordered proteins.

Albert Sales Alba
Universitat de Barcelona, Spain
01/07–31/08/2022
Continuous flow methods to improve intracellular catalysts.

Joseba Uranga Aramburu
UPV/EHU, Spain
01/07–31/08/2022
Analysis and improvement of the execution processes of scientific applications
in DIPC supercomputing systems.

Alfonso Yubero Navarro
Universidad de Zaragoza, Spain
01/07–31/08/2022
Particle physics.

Martín Gutiérrez Amigo
Trinity College Dublin, Ireland
11/07–11/08/2022
PMT covers for Hyper-Kamiokande

Laura Sáenz Díez
Universidad de Cantabria, Spain
11/07–09/09/2022
Controlling light at the nanoscale using classical and quantum effects.

Aitor Echeverría Ibarbia
UPV/EHU, Spain
03/10/2022–Present
Infrastructure Monitoring

Konstantin Todorov
UPV/EHU, Spain
17/10/2022–Present
Analysis and improvement of the execution processes of scientific applications
in DIPC supercomputing systems.

Ganna Mashtaler
Technical University of Munich, Germany
24/10/2022–Present
Implementation and calculation of ab initio electronic couplings in energy transfer processes.

Undergraduate Candidates

Idoia Ugarte Olcoz
UPV/EHU, Spain
12/09/2021–01/07/2022
Double degree of physics and electronic engineering.

Sara Navarro Rodríguez
UPV/EHU, Spain
13/09/2021–08/07/2022
Doped graphene and its electronic properties in general.

Maddi Berasategi Elorza
Universitat Autònoma de Barcelona, Spain
29/09/2021–31/01/2022
Exact exchange functional for hydrogen atom and completely dissociated hydrogen molecule.
Derivation and computational implementation.

Eric Gómez Urreizti
UPV/EHU, Spain
01/10/2021–31/07/2022
Synthesis of cyclic polymers.

Aitor Larrea Mariñelarena
UPV/EHU, Spain
01/01–30/06/2022
Photochemistry.

Ane Zudaire Oses
UPV/EHU, Spain
01/01–30/06/2022
Photochemistry.

Asier Ortiz de Mendibil Jausoro
UPV/EHU, Spain
10/01–08/09/2022
Calculation of electron bands of magnetic materials LaCo2As2 and CaCo2As2 and symmetry analysis.

Julen Galarza Burguete
UPV/EHU, Spain
01/04–30/06/2022
Analysis and improvement of the execution processes of scientific applications
in DIPC supercomputing systems.

Joyce Samantha Romero Jiménez
UPV/EHU, Spain
01/10/2022–Present
Solid State Spectroscopy

Ander Aleson Gurruchaga
UPV/EHU, Spain
11/10/2022–Present
Computational study of aromaticity with descriptors of electronic delocalization.

Master's Degree Students

Arturo Loiselle
UPV/EHU, Spain
13/09/2021–13/05/2022
Enactive cognitive sciences.

Lorea Sánchez Fernández de Larrea
UPV/EHU, Spain
25/10/2021–30/06/2022
Nanoscience and nanotechnology.

Markel González de Chavarri Ylla
UPV/EHU, Spain
01/03–16/06/2022
Development of new density
functional approximations.

Martín Irízar Landa
UPV/EHU, Spain
01/03–01/09/2022
Electronic and spin properties
of graphene nanoribbons.

Carolina Martínez Strasser
UPV/EHU, Spain
24/03–30/06/2022
Spectral properties of a non-Hermitian
diamond chain. Quantum mechanics.

Daniel García Pina
UPV/EHU, Spain
01/04–31/10/2022
Quantum materials.

Asier Enrique Izu Berrade
UPV/EHU, Spain
05/04–15/05/2022
Chemistry.

Special Assignments

Fabienne Barroso Bujans
DIPC Summer Internships

Aitzol García Etxarri
DIPC Transdisciplinary Skills Courses

Aran García-Lekue
DIPC Calls for Young Researchers

Geza Giedke and Thomas Frederiksen
DIPC Colloquia

Marek Grzelczak
DIPC Seminars

Deung-Jang Choi and Nicolás Lorente Palacios
DIPC Courses

Luca Salassa
DIPC Workshops and DIPC Schools

Gustavo Schwartz
Mestizajes program and DIPC
Transdisciplinary Skills Courses

Gender Equality Committee

Amaia Arregi Buldain

Silvia Bonoli

Ricardo Díez Muiño

Luz Fernández Vicente

Maia García Vergniory

Aitzol García Etxarri

Elisa Jiménez Izal

Olatz Leis Esnaola

Irián Sánchez Ramírez

Beatriz Suescun Rodríguez

Visiting Researchers

Long visits

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

Rubén Miguel Ochoa de Zuazola
Hitachi-Cambridge Laboratory, Cambridge, UK
01/01–28/02, 01/03–30/04, 01/05–30/06/2022
Spintronics.

Stefano Scoditti
UNICAL, Cosenza, Italy
08/09/2021–08/03/2022
Design of miniSOG for enhance the photocatalytic properties of riboflavin.

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

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

Wolfgang Schattke
Institut für Theoretische Physik und Astrophysik, CAU, Kiel, Germany
01/01–31/03/2022
Molecular machines on surfaces: nanomechanical properties of small molecules.

Beatrice Bernadette Mascitti
Università degli studi di Padova, Padua, Italy
01/02–31/07/2022
Photocatalytic activation of anticancer drugs.

Laila Abdelfattah Saad Hamam
Faculty of Postgraduate Studies for Advanced Sciences, Beni-Suef University, Beni-Suef, Egypt
02/02–31/07/2022
Science by women.

Oleksiy Roslyak
Fordham University, New York City, NY, USA
23/02–23/03/2022
Electronic excitations in low-dimensional systems.

Oleg Dolgov
Lebedev Physical Institute,
Russian Academy of Science, Moscow, Russia
01/03–31/05/2022
Electronic excitations and superconducting instability in solids.

Fei Gao
Technical University of Denmark,
Lyngby, Denmark
01/03–01/04/2022
Spin transport in transition-metal-based 2-dimensional framework.

Olga Matveeva
Moscow Institute of Physics and Technology,
Center for Photonics and 2D Materials,
Dolgoprudny, Russia
13/03–18/04/2022
Strong coupling of PhPs and molecular vibrations.

Anatolii V. Goncharenko
V.E. Lashkaryov Institute of Semiconductor Physics,
National Academy of Sciences of Ukraine,
Kiev, Ukraine
01/04–31/08/2022
Unconventional plasmonics.

Steen Rasmussen
Center for Fundamental Living Technology,
Odense, Denmark
31/03–15/05/2022
Physics of living materials.

Dmitri Efremov
Leibnitz Institute IFW Dresden,
Dresden, Germany
01/04–01/05/2022
Electronic excitations and superconducting instability in solids.

Roman Kuzian
Institute for Problems of Materials Science
National Academy of Sciences of Ukraine,
Kiev, Ukraine
01/04–29/06/2022
Attosecond electron dynamics in solids.

Jon Marcaide Osoro
Real Academia de Ciencias, Madrid, Spain
01/04–30/06/2022
Molecular structures in the core of SN1987A remnant and Star-planet interaction in LSR J1835+3259.

Karima Benyahia
University of Ain Temouchent,
Belhadj Bouchaib, Algeria
04/04–07/10/2022
Modeling and Study of optoelectronic and excited states of perovskite structures based on energy materials having photovoltaic applications.

Gernot Frenking
Philipps-University Marburg, Marburg, Germany
04/04–31/07/2022
Quantum theoretical studies of the chemical bond.

Mikhail Igorevich Vasilevskiy
Universidade do Minho, Braga, Portugal
04/04–03/07/2022
Photonics and electronics of hybrid structures composed of low-dimensional materials and resonators . Quantum simulation of the energy and charge transport in photosynthesis.

Paula Natalia Abufager
Instituto de Fisica Rosario, Rosario, Argentina
01/05–31/05/2022
Electronic, magnetic and transport properties at the nanoscale.

Giorgio Benedek
Università di Milano-Bicocca, Milano, Italy
01/05–31/05, 03/10–19/11/2022
Dynamics of low-dimensional systems.

Joseph Richard Manson
Clemson University, Clemson, SC, USA
01/05–01/06/2022
Electron-phonon interaction at surfaces.

Oleg V. Prezhdo
University of Southern California,
Los Angeles, CA, USA
01/05–31/07/2022
Excited state dynamics in novel nanoscale materials for optoelectronic applications.

Juan Luis Suárez Sánchez de León
CulturePlex Lab. Western University,
London, Ontario, Canada
01/05–30/06/2022
Complex networks models to approach challenging interdisciplinary problems.

Martin Tomterud
University of Bergen, Bergen, Norway
01/05–31/07/2022
2DMAT: Temperature dependent properties of two dimensional materials.

Román Eugenio Pico
Instituto de Física Rosario, Rosario, Argentina
03/05–30/06/2022
Electronic, magnetic and transport properties at the nanoscale.

Atsushi Ueda
Institute for Solid State Physics,
the University of Tokyo, Chiva, Japan
23/05–23/06/2022
Quantum many body systems.

Anabel Lam Barandela
Instituto de Ciencia y Tecnología de Materiales
Universidad de La Habana, La Habana, Cuba
24/05–23/06/2022
Cyclic Polymers.

Juan Pablo Echeverry Enciso
Universidad de Ibagué, Ibagué-Tolima, Colombia
01/06–30/07/2022
Thermal effects in dielectric response of transition metal dichalcogenides.

Francisco José García Vidal
Universidad Autónoma de Madrid,
Facultad de Ciencias, Madrid, Spain
01/06–31/07/2022
Quantum plasmonics.

Elton Gomes Dos Santos
Higgs Centre for Theoretical Physics,
The University of Edinburgh, Edinburgh, UK
01/06–04/09/2022
Two-dimensional magnetic genome.

Stephanie Louise Yardley
Mullard Space Science Laboratory,
University College London, Holmbury St Mary, UK
01/06–04/09/2022
Solar Physics/Space weather.

Eugene Kogan
Bar-Ilan University, Ramat-Gan, Israel
03/06–02/07/2022
Unoccupied electronic states in MEXENs.

Pawel Harwrylak
University of Ottawa, Ottawa, Canada
06/06–16/07/2022
Nanoplasmonics meets carbononics.

Carmen Mijangos Ugarte
Consejo Superior de Investigaciones Científicas
Instituto de Ciencia y Tecnología de Polímeros,
Madrid, Spain
06/06–05/08/2022
Polymerization reaction in nanoporous materials.

Eduardo V. Ludeña
Instituto Venezolano de Investigaciones Científicas,
Los Salias, Estado Miranda, Venezuela
14/06–14/08/2022
N-representability problem for the 1RDM and 2RDM including excited states.

Dumitru Calugaru
Princeton University, Princeton, NJ, USA
25/06–29/07, 23/09–20/12/2022
Flat phonon bands, gapping flat bands with spin-orbit coupling, thermoelectric effect in TBG.

Michal Bialonczyk
Institute of Theoretical Physics,
Jagiellonian University, Kraków, Poland
01/07–01/09/2022
Full counting statistics of quantum observables.

Aurelia Chenu
University of Luxembourg, Luxembourg
01/07–15/08/2022
Control of open quantum systems.

Gabriel Cwilich
Yeshiva University, New York, NY, USA
01/07–15/08/2022
Network theory, vehicular traffic jams, and transport phenomena.

Adolfo Del Campo Echevarria
University of Luxembourg, Luxembourg
01/07–15/08/2022
Quantum systems and technologies.

Luis A. Elcoro Cengotitabengoa
UPV/EHU, Leioa, Spain
01/07–14/10/2022
ERC Superflat.

Pilar Hernández Gamazo
IFIC, University of Valencia, Paterna, Spain
01/07–31/07/2022
Neutrino physics.

María Ángeles Hernández Vozmediano
Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain
01/07–31/07/2022
Topological matter.

Luis Martín Moreno
Instituto de Nanociencia y Materiales de Aragón, Universidad de Zaragoza, Zaragoza, Spain
01/07–31/07/2022
Theory in nanophotonics.

Vladimiro Mújica Hernández
Arizona State University,
School of Molecular Sciences, Tempe, AZ, USA
01/07–31/12/2022
Chiral-induced spin selectivity effects in molecular environments.

Andrey Vasenko
HSE University, Moscow, Russia
01/07–31/07/2022
Superconductivity in topologically nontrivial materials.

Maxim Kagan
P.L. Kapitza Institute of Physical Problems, Russian Academy of Sciences, Moscow, Russia
19/07–20/08/2022
Anomalous superconductivity and Coulomb correlations in unconventional superconductors.

Olena Klenina
Danylo Halytsky Lviv National Medical University, Lviv, Ukraine
22/07–31/10/2022
Computation of electronic exited states: molecules, aggregates etc.

Oksana Korolyuk
B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Kharkiv, Ukraine
27/07–12/12/2022
Thermophysics applied to the study of novel energy and sustainable materials.

Alejandro González Tudela
Instituto de Física Fundamental, Madrid, Spain
01/08–03/09/2022
Nanophotonics for quantum technologies.

Haoyu Hu
Rice University, Houston, TX, USA
01/08–21/09/2022
Development of flat band theory methods for search of new materials

Nikolay Kabachnik
Lomonosov Moscow State University, Skobeltsyn Institute of Nuclear Physics, Moscow, Russia
01/08–30/09/2022
Two-color multiphoton ionization of atoms and surfaces.

Germán Eduardo Pieslinger
Universidad de Buenos Aires CONICET/IQUIFIB, Buenos Aires, Argentina
01/08/2022–31/08/2023
Bioorthogonal photocatalytic activation of metal-based anticancer prodrugs.

Ziya Aliyev
Institute of Physics, Azerbaijan National Academy of Sciences, Baku, Azerbaijan
05/08–30/09/2022
Materials physics of magnetic topological insulators.

Juan Faustino Aguilera Granja
Universidad Autónoma de San Luis Potosí, San Luis Potosí, México
19/08–19/09/2022
Nanostructures and low dimensional materials.

Maddi Berasategi Elorza
Universitat Autònoma de Barcelona, Barcelona, Spain
01/09–30/11/2022
Exact exchange-correlation functionals for molecular dissociation and electron detachment.

Diego Edmundo Lauer Zegarra
Univesidad Técnico Federico Santa María, Valparaiso, Chile
01/09–03/12/2022
Simulation of first principles of 2D systems.

Ceferino López Fernández
ICMM (CSIC), Madrid, Spain
01/09–30/09/2022
Disorder Photonics and AI.

Daniel Rubén Zerzión
CERN, Meyrin, Switzerland
01/09/2022–28/02/2023
Coherent neutrino collaboration.

Yurii Sitenko
Bogolyubov Institute for Theoretical Physics, NAS of Ukraine, Kiev, Ukraine
04/09/2022–04/01/2023
Quantum effects in the background of topological defect.

Iker Millán Irigoyen
Centro de Investigaciones Energeticas Medioambientales y Tecnologicas, Madrid, Spain
12/09–16/10/2022
Galaxy evolution group.

Ales Paták
Institute of Scientific Instruments, The Czech Academy of Sciences, Brno, Czech Republic
12/09–10/10/2022
Ab initio study of angle-resolved spectroscopy of few-layer graphene.

Luis Alberto Montero Cabrera
Universidad de La Habana,
Facultad de Química, La Habana, Cuba
16/09–15/11/2022
Artificial Inlelligence applied to spectroscopic properties of molecules.

Jon Zapata Muñoz
DigiPen Institute of Technology Europe-Bilbao, Bilbao, Spain
19/09–19/11/2022
Cosmology.

Chizoba May Obele
Nnamdi Azikiwe University, Anambra State, Awka, Nigeria
22/09/2022–19/03/2023
Development of non toxic antifouling coating susing nanotubes.

Jonah Herzog-Arbeitman
Princeton University, Princeton, NJ, USA
26/09–30/11/2022
Flat band topology and heavy fermion models.

Ursula Fernanda Salazar Roggero
Unicamp, Campinas, Sao Paulo, Brazil
26/09–31/12/2022

Julio Alonso Martín
Facultad de Ciencias, Universidad de Valladolid, Valladolid, Spain
01/10–30/11/2022
Interaction of small molecules with layered materials.

Nicolas Regnault
LPENS, École normale supérieure de Paris
and CNRS, Paris, France
01/10/2022–28/02/2023
ERC_AdG SUPERFLAT.

Aleksander Bach Lorentzen
Technical University of Denmark,
Lyngby, Denmark
05/10–15/11/2022
Nanostructured nanoporous graphene.

Jauvert Ludovic
CNRS and Université de Bordeaux,
Bordeaux, France
06/10–07/12/2022
Basque and IKUR quantum science
and technology workshop.

Chunli Huang
Los Alamos National Lab., Los Alamos, NM, USA
10/10–09/12/2022
Superconductivity and spin-transport
in two dimensional materials.

Eusebio Jesús Rodríguez Fernández
Universidad de Sevilla, Sevilla, Spain
16/10–16/11/2022
Spin dynamics in curved spaces.

Juan Felipe Huan Lew Yee
Facultad de Química,
Universidad Nacional Autónoma de México,
Ciudad de México, Mexico
18/10–25/11/2022
Coupling of the local density fit to Piris
natural orbital functionals.

Aaron Chew
Princeton University, Princeton, NJ, USA
31/10–28/12/2022
Interactions in twisted bilayer graphene in flux.

Raffaele Resta
Istituto Officina dei Materiali,
CNR; University of Trieste, Trieste, Italy
01/11/2022–31/01/2023
Geometry and topology
in condensed matter physics.

Leonid Sandratskii
Institute of Physics of the Czech Academy
of Sciences, Praga, Czech Republic
01/11–30/11/2022
Spin-orbit coupling effects in the magnetism
of 5f-electron systems.

Stefano Scoditti
UNICAL, Arcavacata CS, Cosenza, Italy
15/11–15/12/2022
Photocatalysis of metal complexes.

Marco Tuccio
Università di Torino, Torino, Italy
22/11–23/12/2022
Surface DNA hybridization r-ates.

Short visits

Tomas Neuman
ISMO, CNRS, Orsay, France
23/01–27/01/2022
Theory of scattering-type near-field microscopy
and infrared spectroscopy.

Daniel Gallego Fuente
Universidad Autónoma de Madrid, Madrid, Spain
30/01–05/02/2022
ERC StG.

Dimas García de Oteyza Felderman
CINN, CSIC-UNIOVI-PA, El Entrego, Spain
02/02–04/02, 16/02–18/02, 09/03–11/03,
16/03–18/03, 30/03–01/04, 20/04–22/04/2022
On-surface synthesis of functional molecular
materials on surfaces.

Alexander Golubov
University of Twente, Enschede, The Netherlands
02/02–07/02/2022
Superconductor/topological insulator
hybrid structures.

Mads Brandbyge
Technical University of Denmark,
Kongens Lyngby, Denmark
01/03–08/03, 20/10–28/10/2022
Spin transport in transition-metal-based
2-dimensional framework.

Antonio Hernando Grande
Instituto de Magnetismo Aplicado,
Universidad Complutense de Madrid, Madrid, Spain
09/03–13/03, 07/10–17/10, 27/11–11/12/2022
Effect of magnetic fields on gating
of neuron channels.

Alessandro De Martino
University of London, London, UK
14/03–19/03/2022
Effects of spin-orbit coupling on transport
properties of graphene pn-junctions.

Diego Frustaglia
Universidad de Sevilla, Sevilla, Spain
15/03–19/03/2022
Spin dependent quantum transport.

David Alonso Monge
University of Oxford, Oxford, UK
16/03–18/03/2022
Numerical simulations in cosmology.

Isabel Márquez Pérez
Instituto de Astrofísica de Andalucia,
Granada, Spain
21/03–25/03/2022
Active galaxies in J-PAS.

Siddhartha Gurung López
Observatorio Astronómico
de la Universidad de Valencia, Paterna, Spain
29/03–01/04/2022
Ly-alpha emitters detection in J-PAS.

Alberto Torralba Torregrosa
Observatorio Astronómico
de la Universidad de Valencia, Paterna, Spain
29/03–01/04/2022
Lyman-alpha Emitters in J-PAS.

Susana Elizabeth Pedrosa
Institute for Astronomy and Space Physics,
Caba, Argentina
06/04–09/04/2022
Physics of galaxy formation.

Erez Gilad
Ben-Gurion University of the Negev, Israel
20/04–30/04/2022
Ess Neutron Background Calculations.

Joshua Edward Renner
IGFAE / Universidad de Santiago de Compostela,
Santiago de Compostela, Spain
20/04–23/04/2022
GanESS.

Alberto Otero de la Roza
Universidad de Oviedo,
Facultad de Química, Oviedo, Spain
21/04–23/04/2022
Metastable and active carbon-based materials
for the storage and management of clean
energy–Novel Physico-chemical
strategies (MACMAT).

Wojciech Gawelda
IMDEA-Nanociencia, Universidad Autónoma de
Madrid, Madrid, Spain
28/04–29/04/2022
New era in structural dynamics research:
why will X-ray free electron lasers revolutionize
the X-ray science?

Vitaliy Goryashko
Uppsala University, Uppsala, Sweden
29/04–06/05/2022
Nanooptics of magnetic materials.

Salvador Miret Artés
Instituto de Física Fundamental,
CSIC, Madrid, Spain
03/05–06/05, 24/05–27/05,
03/10–14/10, 08/11–13/11/2022
Electron phonon coupling.

Carlos Andrés Peniche Covas
Facultad de Química,
Universidad de La Habana, La Habana, Cuba
07/05–21/05/2022
Polymers for biomedical applications.

Ángel Martín Pendás
Universidad de Oviedo, Oviedo, Spain
09/05–14/05/2022
Open quantum systems and local spin.

Viktor Chikan
Kansas State University, Manhattan, NY, USA
12/05–14/05/2022
Triggering molecular transport
via pulse magnetic field.

David Nicolás Laroze Navarrete
Universidad de Tarapacá, Arica, Chile
15/05–22/05/2022
Chaotic dynamics in synthetic antiferromagnetic
nano-particles.

María Navarro Gastiasoro
Institute for Complex Systems,
Consiglio Nazionale delle Ricerche, Rome, Italy
17/05–26/05/2022
Superconductivity mediated by
soft ferroelectric modes.

Richard Douglas Robinson
Cornell University, Ithaca, NY, USA
20/05/2022
Magic from magic-sized clusters: reversible
isomerization and centimeter-length hierarchical
self-organization.

Cesar Aurelio Herreño Fierro
Universidad Distrital Francisco José de Caldas,
Bogotá, Colombia
24/05–27/05/2022
Optical response of metallic nanostructures.

Urko Petralanda Holguín
UPV/EHU, Leioa, Spain
26/05–27/05/2022
Domain walls in two-dimensional ferroelectric
monochalcogenides.

Oskar Vafek
Florida State University and National High
Magnetic Field Institute, Tallahassee, FL, USA
27/05–09/06/2022
Theory of moire graphene.

Konstantin Bliokh
RIKEN, Saitama, Japan
31/05–10/06/2022
Momentum and angular momentum
of classical waves.

Inés Martínez Martín
Centro Nacional de Investigaciones
Cardiovasculares, Madrid, Spain
06/06–17/06/2022
Molecular dynamics of titin domain Ig 21.

Michael Thoss
Institute of Physics, University of Freiburg,
Freiburg, Germany
11/06–18/06/2022
Quantum transport in molecular junctions.

Daniel Rubén Zerzión
ESS-Lund, Lund, Sweden
11/06–16/06/2022
Discussions and analysis of the next years work
towards the design, construction, installation and
data taking and analysis research of a high pressure.

Andrey Postnikov
Université de Lorraine Laboratoire de Chimie
et Physique – Approche Multi-Echelles
des Milieux Complexes, Metz, France
12/06–18/06/2022
Electronic structure and vibrations
in semiconductors.

Pere Alemany i Cahner
Universitat de Barcelona, Barcelona, Spain
13/06–17/06/2022
Development of a web interface for Cosymlib:
a python library to analyze the shape
and symmetry of molecular structures.

Talat Shahnaz Rahman
University of Central Florida, Orlando, FL, USA
18/06–01/07/2022
Theoretical and computational investigations
of transport, magnetic and optical properties of
functional nanomaterials.

Pavel Jelínek
Institute of Physics of the Czech Academy
of Sciences, Praga, Czech Republic
20/06–08/07/2022
Low-dimensional molecular systems.

Aaron Chew
Princeton University, Princeton, NJ, USA
25/06–23/07/2022
Interactions in twisted bilayer graphene in flux.

Frank Titus Avignone
University of South Carolina, Columbia, SC, USA
01/07–04/07/2022
Contributions to NEXT experiment.

Jonah Herzog-Arbeitman
Princeton University, Princeton, NJ, USA
08/07–31/07/2022
Topological insulators.

Karolina Slowik
Institute of Physics Nicolaus Copernicus University in Torun, Torun, Poland
09/07–22/07/2022
Investigating electro-optical properties of graphene nanoflakes with adatoms.

Rafael María Gutiérrez Salamanca
New York University Abu Dhabi, Abu Dhabi, United Arab Emirates
10/07–01/08/2022
Neutrinos (Complexity and Biophysics).

Marta Losada
New York University Abu Dhabi, Abu Dhabi, United Arab Emirates
10/07/2022–01/08/2022
Neutrinos.

Marta Pelc
Institute of Physics Nicolaus Copernicus University in Torun, Torun, Poland
10/07–22/07/2022
Investigating electro-optical properties of graphene nanoflakes with adatoms.

Charles Mark Lewis
University of Chicago, Chicago, IL, USA
11/07–15/07/2022
The Next generation of CEvNS measurements.

Javier García de Abajo
ICFO-Instituto de Ciencias Fotónicas, Castelldefels, Spain
16/07–30/07/2022
Plasmonics in atomically thin crystalline silver films.

José Ángel Hernando Morata
Instituto Galego de Antas Enerxías, Universidad de Santiago de Compostela, Santiago de Compostela, Spain
17/07–30/07/2022
NEXT.

Olga Movilla Miangolarra
University of California, Irvine, CA, USA
18/07–15/08/2022
Advances in shortcuts to adiabaticity and quantum control.

Francesca Ferlaino
Institute for Experimental Physics
University of Innsbruck, Innsbruck, Austria
25/07–03/08/2022
Novel quantum phases in ultracold dipolar gases.

Jinxiu Zhou
Centro Joxe Mari Korta, Donostia/San Sebastián, Spain
25/07–07/08/2022
New Helix polymer based on unnatural densely substitute proline.

Almudena Arcones Segovia
Technische Universität DarmstadtInstitut für Kernphysik, Darmstadt, Germany
26/07–30/07/2022
Nuclear physics, nuclear astrophysics neutrino physics.

Achim Schwenk
Technische Universität DarmstadtInstitut für Kernphysik, Darmstadt, Germany
26/07–30/07/2022
Nuclear physics, nuclear astrophysics neutrino physics.

María Eugenia Sandoval Salinas
Universidad de Alicante, San Vicente del Raspeig, Spain
01/08–27/08/2022
Photophysical properties of multicromophoric systems.

Orlando Tapia
University of Uppsala
Department of Chemistry - BMC, Uppsala, Sweden
01/08–15/08/2022
Foundations of Molecular Quantum Mechanics.

Norio Kawakami
Kyoto University, Kyoto, Japan
08/08–16/08/2022
Investigation of the load and spin transport properties in low dimensional systems, highly correlated systems and superconductors.

Amos Martínez García
Nature Springer, London, UK
08/08–10/08/2022
Nanophotonics.

Pei Chin Won
Nature Springer, London, UK
08/08–10/08/2022
Nanophotonics.

Nicolas Regnault
Princeton University, Princeton, NJ, USA
16/08–19/08/2022
Hilbert space fragmentation, Topological Phonon Database (ERC).

Xi Dai
Hong Kong University of Science and Technology, Hong Kong, China
18/08–21/08/2022
Topological materials.

Martina Soldini
University of Zurich, Zurich, Switzerland
22/08–15/09/2022
Correlations in topological materials.

Arthur Ernst
Institute of Theoretical Physics, Johannes Kepler University Linz, Linz, Austria
29/08–14/09/2022
Electronic and magnetic properties of 2D materials.

Max Mende
Technische Universität DresdenInstitut für Festkörper- und Materialphysik, Dresden, Germany
10/09–24/09/2022
Synchrotron-based studies of 4f-materials.

Georg Poelchen
European Synchrotron Radiation Facility, Grenoble, France
10/09–20/09/2022
Synchrotron-based studies of 4f materials.

Susanne Schulz
Institute for Solid State and Materials Physics, Dresden, Germany
10/09–24/09/2022
Synchrotron-based studies of 4f-materials.

Sergio Carbajo
SLAC National Accelerator Laboratory, Stanford University, Stanford, CA, USA
11/09–13/09/2022
Prospects on nonequilibrium (Bio)chemistry via THz-driven water.

Agata Wislocka
University of Vienna, Institut for Astrophysics, Wien, Austria
12/09–23/09/2022
Cosmology.

Alexander Yaresko
Max Planck Institute for Solid State Research, Stuttgart, Germany
19/09–30/09/2022
Magnetic dichroism in layered intermetallic compounds.

Guinevere Kauffmann
Max Planck Institute for Astrophysics, Garching, Germany
24/09–15/10/2022
Constraining the nature of massive stars in the most active galactic bulges.

Simon White
Max Planck Institute for Astrophysics, Garching, Germany
24/09–16/10/2022
Cosmic structure formation.

José Álvarez Cuervo
Universidad de Oviedo, Oviedo, Spain
25/09–30/09/2022
Hiperbolic nanooptics.

Christian Lanza García
Universidad de Oviedo, Oviedo, Spain
25/09–30/09/2022
Hiperbolic nanooptics.

Rolf Heid
Karlsruhe Institute of Technology,
Eggenstein-Leopoldshafen, Germany
26/09–28/09/2022
Electron-phonon interaction from first principles.

Miguel Ángel Jiménez Herrera
UPV/EHU, Donostia/San Sebastián, Spain
01/10–16/10/2022
Topological properties of synthetic
two-dimensional lattice systems.

Jon Lasa Alonso
CSIC-UPV/EHU, Donostia/San Sebastián, Spain
01/10–16/10/2022
Antidual particles and their properties.

Jhon Wilfer González Salazar
Universidad Técnica Federico Santa María,
Valparaiso, Chile
04/10–14/10/2022
Electronic and magnetic properties of 2D
materials and small clusters.

Steen Rasmussen
Center for Fundamental Living Technology,
Odense, Denmark
04/10–11/10/2022
Physics of living materials.

Luca Sala
University Observatory, Faculty of Physics,
Ludwig-Maximilians-Universität München,
Munich, Germany
04/10–28/10/2022
Scheduled secondment according
to BiD4BESt ITN plan.

Iván Ezequiel López
Università di Bologna, Bologna, Italy
08/10–31/10/2022
Secondement of ITN Bid4Best network -
work on "properties of AGN host galaxies".

Chervin Laporte
ICCUB, Facultad de Física, Barcelona, Spain
13/10–15/10/2022
The milky way as a galaxy formation
and dark matter lab.

David Izquierdo Villalba
Universtiá degli Studi di Milano Biocca, Milano, Italy
19/10–22/10/2022
Black hole growth and spin evolution.

Fei Gao
Technical University of Denmark, Lyngby, Denmark
20/10–26/10/2022
Spin transport in transition-metal-based
2-dimensional framework.

Stephen Power
School of Physical Sciences, Dublin, Ireland
20/10–22/10/2022
PhD Defence.

Alexandre Reily Rocha
Instituto de Física Teórica, São Paulo State
University, São Paulo, Brazil
21/10–25/10/2022
Electron phonon interactions and transport
in disordered systems.

Nicolas Fefeu
University of Bordeaux, Bordeaux, France
24/10–28/10/2022
2D nanophotonics.

Ramón Aguado Sola
Instituto de Ciencia de Materiales de Madrid,
Madrid, Spain
02/11–05/11/2022
Theory of quantum materials and solid state
quantum technologies.

Daniela Galárraga Espinosa
Max-Planck-Institute for Astrophysics,
Garching bei München, Germany
08/11–11/11/2022
Exploring galaxy connectivity.

Enrico Garali
Max Planck Institute for Astrophysics,
Garching bei Muenchen, Germany
08/11–11/11/2022
Evolution of the high-redshift galaxies
and reionization.

Herbert Fertig
Indiana University, Bloomington, IN, USA
09/11–13/11/2022
Studies of topological condensed matter.

Luisa Cifarelli
University of Bologna and INFN, Bologna, Italy
10/11–12/11/2022
DIPC Advisory Committee.

Christophe Rossel
IBM Research-Zurich, Rüschlikon, Switzerland
10/11–12/11/2022
DIPC Advisory Committee.

Henrique Rubira
Technique University Munich,
Garching bei München, Germany
10/11–11/11/2022
Full-shape BOSS constraints on dark matter
interacting with dark radiation and lifting
the S8 tension.

Petra Rudolf
University of Groningen, Zernike Institute for
Advanced Materials, Groningen, Netherlands
10/11–12/11/2022
DIPC Advisory Committee.

Philipp Strasberg
Quantum Information Group, Facultad de
Ciencias, UAB, Bellaterra, Barcelona Spain
15/11–19/11/2022
Quantum nonequilibrium statistical mechanics.

Kristoffer Reinholt Thomsen
University of Southern Denmark,
Odense, Denmark
24/11–20/12/2022
Open questions in protocell design research.

Daria Szewczyk
Universidad Autonoma de Madrid, Madrid, Spain
01/12–04/12/2022
Heat capacity features of the mixed lead halide
perovskites of the MAPbX3 type.

Ming-Chiang Chang
National Chung-Hsing University, Taichung, Taiwan
05/12–14/12/2022
Uhlmann Phase of GGE.

Andrew Jamieson
Max-Planck Institute for Astrophysics,
Garching, Germany
06/12–17/12/2022
Nachine learning in cosmology.

Administration and Services

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Head of Outreach & Communication

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Head of Finance & Accounting
and R+D+i Project Management

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Head of Supercomputing Center

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

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End of contract 15/11/2022

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Security, Web & Networks

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HPC Resources
End of contract 15/11/2022

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Seminars

1 Shortcuts to Adiabaticity
13/01/2022
Xi Chen
UPV/EHU, Donostia/San Sebastián, Spain

2 Using synchrotron-based X-ray techniques to direct the design of improved metallic devices for biological applications
03/02/2022
Carlos Sánchez Cano
DIPC, Donostia/San Sebastián, Spain

3 Primordial black holes as dark matter candidates
11/02/2022
Joaquín Sureda Hernández
DIPC, Donostia/San Sebastián, Spain

4 Size and composition effects in heterogeneous catalysis through the electronic structure insight
17/02/2022
Elisa Jiménez-Izal
UPV/EHU, DIPC, Donostia/San Sebastián, Spain

5 Cosmic kite: Auto-encoding the Cosmic Microwave Background
25/02/2022
Martín de los Ríos
Instituto de Física Teórica, UAM, Madrid, Spain

6 Quantum and Quantum-Inspired Algorithms for Matter and Beyond
03/03/2022
Román Orús Lafort
DIPC, Multiverse Computing, Donostia/San Sebastián, Spain

7 Basi(c)s of Nonequilibrium Statistical Mechanics–Made Simple
07/03/2022
Philipp Strasberg
UAB, Barcelona, Spain

8 Chemical stability of zigzag edges in carbon nanostructures
17/03/2022
Dimas García de Oteyza Felderman
CINN, CSIC-UNIOVI-PA, Oviedo, Spain

9 Some practicalities of cosmological photometric redshift datasets
18/03/2022
Davíd Alonso Monge
University of Oxford, Oxford, UK

10 The presence and impact of outflows at the lowest end of nuclear activity
24/03/2022
Isabel Márquez Pérez
IAA-CSIC, Granada, Spain

11 Exploration of Topological Band Structures using Deep Learning
25/03/2022
Vittorio Peano
Max Planck Institute for the Science of Light, Erlangen, Germany

12 Ultrastrong light-matter coupling in materials: From plasmonic supercrystals to ferroelectrics
28/03/2022
Stephanie Reich
Freie Universitaet Berlin, Berlin, Germany

13 High pressure gaseous TPCs for neutrino physics
31/03/2022
Francesc Monrabal Capilla
DIPC, Donostia/San Sebastián, Spain

14 Shortcuts to adiabaticity, a tool for quantum science and technology
01/04/2022
Juan Gonzálo Muga
UPV/EHU, Donostia/San Sebastián, Spain

15 Assembly and evolution of minimal living materials
08/04/2022
Steen Rasmussen
University of Southern Denmark, Odense, Denmark

16 XDM-corrected density-functional theory for crystal structure prediction
22/04/2022
Alberto Otero de la Roza
Universidad de Oviedo, Oviedo, Spain

17 DIPC Community Seminars: Synthesis and applications of cyclic polymers
28/04/2022
Fabienne Barroso Bujans
DIPC, Donostia/San Sebastián, Spain

18 New era in structural dynamics research:
why will X-ray Free Electron Lasers revolutionize the X-ray Science?
29/04/2022
Wojciech Gawelda
IMDEA-Nanociencia, UAM, Madrid, Spain

19 Triggering molecular transport via pulse magnetic fields
13/05/2022
Viktor Chikan
Kansas State University, Manhattan, KS, USA

20 Atoms in molecules from an open systems perspective
13/05/2022
Angel Martín Pendás
Universidad de Oviedo, Oviedo, Spain

21 Chitosan based systems for biomedical and pharmaceutical applications
19/05/2022
Carlos Andrés Peniche Covas
Facultad de Química, Universidad de La Habana, La Habana, Cuba

22 Magic from magic-sized clusters:
reversible isomerization and centimeter-length hierarchical self-organization
20/05/2022
Richard Robinson
Cornell University, New York City, NY, USA

23 Superconductivity mediated by soft ferroelectric modes
24/05/2022
Maria Navarro Gastiasoro
ISC-CNR, Sapienza University of Rome, Rome, Italy

24 Mental Health Issues and the Ethics of Care in Research Intensive Institutions
24/05/2022
Erin Huner
Ivey Business School, London, Canada

25 DIPC Community Seminars: Spins on surfaces for quantum technology
26/05/2022
Deung-Jang Choi
DIPC, Donostia/San Sebastián, Spain

26 Domain walls in 2D monochalcogenide ferroelectrics
27/05/2022
Urko Petralanda Holguín
UPV/EHU, Donostia/San Sebastián, Spain

27 Narrow bands in magnetic field and strong-coupling Hofstadter spectra
07/06/2022
Oskar Vafek
National High Magnetic Field Lab, Florida State University, Tallahassee, FL, USA

28 DIPC Community Seminars: Photophysics of organic materials from a computational perspective
09/06/2022
Claire Tonnelé
DIPC, Donostia/San Sebastián, Spain

29 Quantum Transport in Molecular Junctions
13/06/2022
Michael Thoss
University of Freiburg, Freiburg, Germany

30 Adsorption of atoms (alkali metals) and molecules (atmospheric gases) on graphene-like monolayers: DFT results
15/06/2022
Andrei Postnikov
University de Lorraine, Metz, France

31 Visualizing the renormalization group flows with tensor network
22/06/2022
Atsushi Ueda
University of Tokyo, Tokyo, Japan

32 Quantum Materials and Devices Seminar: Quantum transport with cold atomic gases
22/06/2022
Thierry Giamarchi
Ecole de Physique, University of Geneva, Geneva, Switzerland

33 DIPC Community Seminars: Light matter interactions at the nanoscale
23/06/2022
Aitzol García Etxarri
DIPC, Donostia/San Sebastián, Spain

34 Designing materials at the nanoscale
30/06/2022
Pawel Hawrylak
University of Ottawa, Ottawa, Canada

35 The Next Generation of CEvNS Measurements
12/07/2022
Mark Lewis
University of Chicago, Chicago, IL, USA

36 Chiral effective field theory for dark matter direct detection
27/07/2022
Achim Schwenk
TU Darmstadt, Darmstadt, Germany

37 Inside Nature journals: An editors view
09/08/2022
Amos Martínez García
Editor at Nature Materials, London, UK

38 Quantum Materials and Devices Seminar: Non-Hermitian quantum phenomena in correlated systems
10/08/2022
Norio Kawakami
Kyoto University, Kyoto, Japan

39 Nanophotonics for quantum technologies
11/08/2022
Alejandro González-Tudela
IFF-CSIC, Madrid, Spain

40 2nd Seminar of Internship Students at DIPC
30/08/2022
DIPC, Donostia/San Sebastián, Spain

41 Prospects on Nonequilibrium (Bio)chemistry via THz-driven Water Dynamics Probed by Novel X-ray/Electron Sources
12/09/2022
Sergio Carbajo García
UCLA, SLAC National Accelerator Laboratory, Los Angeles, CA, USA

42 HR-pyPopStar: New tool to create single stellar population spectra and how to use them to analyse galaxies
30/09/2022
Iker Millán Irigoyen
CIEMAT, Madrid, Spain

43 DIPC Community Seminars: Hyperbolic light
06/10/2022
Alexey Nikitin
DIPC, Donostia/San Sebastián, Spain

44 DIPC Community Seminars: From neutrinoless double beta decay nuclear reactions to supramolecular chemistry
20/10/2022
Fernando P. Cossío
UPV/EHU, DIPC, Donostia/San Sebastián, Spain

45 Science without Frontiers? Cosmopolitanism and national interests in the sciences in times of peace and in times of war
20/10/2022
Robert Fox
HSMT, University of Oxford, Oxford, UK

46 Magnetic anisotropy and magnetic ordering of transition-metal phosphorus trisulfides
21/10/2022
Cheol-Hwan Park
Seoul National University, South Korea, DIPC, Donostia/San Sebastián, Spain

47 Using Machine Learning methods to obtain the properties of water
24/10/2022
Alexandre Reily Rocha
IFT, UNESP, São Paulo, Brazil

48 Synthesis and characterization of inorganic perovskite quantum dots for photovoltaic applications
25/10/2022
Laila Saad
Faculty of Postgraduate Studies for Advanced Sciences, Beni-Suef University, Beni-Suef, Egypt

49 New tools in our quantum transport toolbox
26/10/2022
Mads Brandbyge
DTU Physics, Lyngby, Denmark

50 Public private partnerships for large scientific projects
28/10/2022
Miguel Ángel Carrera Astigarraga
Added Value Solutions, Spain

51 Yu-Shiba-Rusinov subgap excitations in hybrid superconductor/semiconductor nanowires containing quantum dots
03/11/2022
Ramón Aguado Sola
ICMM-CSIC, Madrid, Spain

52 A fierce new challenge: unveiling the connection between the first galaxies and reionization
09/11/2022
Enrico Garaldi
Max Planck Institute for Astrophysics, München, Germany

53 DIPC Community Seminars: Electronic structure investigations at Nanophysics Lab in San Sebastian
10/11/2022
Frederik Schiller
CSIC-UPV/EHU, Donostia/San Sebastián, Spain

54 Quantum Geometric Dipole in Collective Excitations
11/11/2022
Herbert Abraham Fertig
Indiana University, Bloomington, IN, USA

55 Full-shape BOSS constraints on dark matter interacting with dark radiation and lifting the S8 tension
11/11/2022
Henrique Rubira
TUM, München, Germany

56 Deep insight into the electronic structure of organic single crystal: rubrene
16/11/2022
Satoshi Kera
Institute for Molecular Science, Okazaki, Japan

57 Classicality without decoherence: A new approach?
18/11/2022
Philipp Strasberg
UAB, Barcelona, Spain

58 Optical adventures with correlated matter – quantum simulation, optical probing, and more
24/11/2022
Tobias Grass
DIPC, Donostia/San Sebastián, Spain

59 Heat capacity features of the mixed lead halide perovskites of the MAPbX3 type
02/12/2022
Daria Szewczyk
INTiBS, Wrocław, Poland, Low Temperature Laboratory, UAM, Madrid, Spain

60 Characterisation of cell motility through a bioimage analysis perspective
22/12/2022
Estíbaliz Gómez de Mariscal
Instituto Gulbenkian de Ciência, Oeiras, Portugal

Workshops

Other Workshops

Conference on Quasielastic Neutron Scattering and Workshop on Inelastic Neutron Spectrometers (QENS/WINS 2022)

May 23-27, 2022
Live streamed and in-person
Miramar Palace, Donostia/San Sebastián
http://qens-wins2022.dipc.org/

Organizing Committee
Arantxa Arbe (CFM-MPC)
Juan Colmenero (CFM-MPC)
Karmela Alonso (DIPC)
Ane Iturriza (MPC)
Amaia Iturrospe (CFM)
Marta López (MPC)
Jon Maiz (MPC)
Paula Malo de Molina (MPC)
Carmen Martin (DIPC)

The celebration of QENS/WINS 2022 constituted the 15th Edition of the QENS series and the 10th of the WINS workshops.

Following the spirit of QENS Conferences since 1992, the main purpose of QENS was to cover the broad spectrum of scientific activities related with the investigation of material dynamics using quasi-elastic neutron scattering techniques (accessing both, frequency and time domains). QENS 2022 offered a platform for discussion and exchange of scientific ideas among the experts in this field, and a general overview to newcomers about the capabilities of QENS in exploring atomic and molecular motions and relaxation processes of novel materials. As a novelty, this QENS edition explored and exploited the potential synergies between different methods (including experimental techniques and simulations, but always with QENS in the spotlight), in order to face diverse scientific challenges emerging in different research fields.

WINS --the 10th Workshop on Inelastic Neutron Spectrometers– covered innovative aspects of neutron instrument design. Progresses on new spectrometer projects were presented. As in previous editions, the theme of "New idea, New concept, New design, New instrumentation for New sciences" was followed. New developments in the application of polarization analysis, magnetic field, pressure, or improvements in sample environments for soft matter systems were covered. Software for data acquisition, analysis and instrument simulation were also part of the program. In analogy with the spirit of QENS 2022, the synergy with complementary methods –in this case mainly with advanced simulations and extensive Monte Carlo simulations—was emphasized.

Along QENS/WINS 2022, 45 invited talks were given, including 4 plenaries and 11 keynotes. Different topics were covered by the QENS conference, from energy-related investigations to the biological world, passing through polymers and soft matter in general, water and other liquids, magnetism and functional materials. Remarkable was the notable participation of young scientists in the event. To stimulate young researchers, two works were awarded with the QENS/WINS Poster Prizes. During the Conference, the 50th anniversary of the birth of the Neutron Spin Echo technique was celebrated with a talk delivered by its inventor, Prof. Feri Mezei.

Invited Speakers
Ken Andersen (ORNL, USA)
Antonio Faraone (NIST, USA)
Sandrine Lyonnard (CEA Grenoble, France)
Kristine Niss (Roskilde University, Denmark)
Robert Bewley (ISIS, UK)
Alessandro Cunsolo (Brookhaven National Laboratory, USA)
Bjorn Fåk (ILL, Grenoble, France)
Bernhard Frick (ILL, Grenoble, France)
Robert Leheny (The Johns Hopkins University, Baltimore, USA)
Bing Li (Chinese Academy of Sciences, Shenyang, China)
Ferenc Mezei (Mirrotron, Hungary)
Christof Niedermayer (PSI, Switzerland)
Gabriele Sala (SNS, USA)
Andreas Stadler (JCNS, Jülich, Germany)
Fan Yang (German Aerospace Center, Köln, Germany)
Frederico Alabarse (Elettra, Trieste, Italy)
Katrin Amann-Winkel (Max-Planck Institute for Polymer research & JGU Mainz, Germany)
Antonio Benedetto (University College Dublin, Ireland & Roma Tre University, Italy)
Marcella Cabrera Berg (JCNS, Jülich, Germany)
Karin J. Bichler (Louisiana State University, Baton Rouge, USA)
Wangchun Chen (NIST,USA)

Xiangquiang Chu (China Academy of Engineering Physics, China)
Francoise Damay (LLB, Saclay, France)
Arnaud Desmedt (University of Bordeaux, France)
Bela Farago (ILL, Grenonble, France)
Fabrizia Foglia (University College London, UK)
Johanna Jochum (TUM, Garching, Germany)
Yukinobu Kawakita (JPARC, Japan)
Maiko Kofu (JPARC, Japan)
Margarita Kruteva (JCNS, Jülich, Germany)
Chris Ling (University of Sydney, Australia)
Benqiong Liu (CMRR, China)
Paula Malo de Molina (MPC, San Sebastian, Spain)
Eugene Mamontov (ORNL, USA)
Lucile Mangin-Thro (ILL, Grenoble, France)
Takatsugu Masuda (University of Tokyo, Japan)
Koichi Mayumi (University of Tokio, Japan)
Gøran Nilsen (ISIS, UK)
Marie Plazanet (University Grenoble Alpes, France)
Timmy Ramirez-Cuesta (ORNL, USA)
Felix Roosen-Runge (Lund University, Sweden)
Margarita Russina (HMI, Berlin, Germany)
Rasmus Toft-Petersen (ESS, Sweden)
Gregory Tucker (ESS, Sweden)
Maximillian Wolff (Uppsala University, Sweden)
Jean Marc Zanotti (LLB, Saclay, France)

Topological Photonics Workshop 2022 (TopoPhoto2022)

June 01-03, 2022
DIPC, Donostia/San Sebastián
http://topophoto2022.dipc.org

Organizing Committee
Aitzol García-Etxarri (DIPC)
Paloma Arroyo Huidobro (Instituto de Telecomunicações, IST-University of Lisbon)

This workshop was aimed at gathering a critical mass of people working in the vibrant area of Topological Photonics as well as topology in other wave phenomena.

The conference objectives were achieved very successfully. The conference was a success both from the scientific and the social point of view.

Invited Speakers
Alexander Khanikaev (The City College of NY, USA)
Mohamed Hafezi (University of Maryland, USA)
Andrea Alu (The City College of NY, USA)
Shanhui Fan (Stanford Universtiy, CA, USA)
Mário G. Silveirinha (Instituto de Telecomunicações, IST-University of Lisbon, Portugal)
Konstantin Bliokh (Riken, Japan)
Maia Garcia-Verniory (DIPC, Spain)
Ewold Verhagen (AMOLF, The Netherlands)
Alejandro González-Tudela (CSIC, Spain)
Pedro David García (ICN2, Spain)
Alberto Amo (CNRS, Université de Lille, France)
Vincenzo Giannini (CSIC, Spain)
Sebastian Huber (ETH, Switzerland)
Beatriz Olmos (University of Tübingen, Germany)

International Conference on Reduced Density Matrix Theory for Quantum Many-Fermion Systems (RDM2022)

June 15-17, 2022

Miramar Palace, Donostia/San Sebastián

http://rdm2022.dipc.org/

Organizing Committee

Mario Piris (DIPC, UPV/EHU, Ikerbasque)

Christian Schilling (LMU Munich)

David Mazziotti (University of Chicago)

The interdisciplinary workshop brought together experts from the quantum sciences, in particular quantum chemistry and quantum information theory, to deepen into the conceptual aspects of the interaction of many-fermion quantum systems. The aims were to discuss recent ideas and identify open challenges related to energy determination and properties of interacting fermions in terms of reduced density matrices (RDM). The workshop explored the theory and applications of ground and excited states, as well as time-dependent processes.

Invited Speakers

Eduardo V. Ludeña (Instituto Venezolano de Investigaciones Científicas, Caracas, Venezuela)

Albert Eugene DePrince III (Florida State University, USA)

Thierry Deutsch (University Grenoble Alpes, CEA, IRIG-MEM, Grenoble, France)

Julia Liebert (LMU Munich, Germany)

Robertus van Leeuwen (University of Jyväskylä, Finland)

Lexin Ding (LMU Munich, Germany)

Paul Andrew Johnson (Université Laval, Quebec, Canada)

Iva Brezinova (Institute for Theoretical Physics, TU Wien, Austria)

Eduard Matito (DIPC, Spain)

Ion Mitxelena (Faculty of Chemistry, UPV/EHU, Spain)

Joshua Hollett (University of Winnipeg, Canada)

Klaas J. H. Giesbertz (Vrije Universiteit Amsterdam, Netherlands)

Tomasz Maciazek (University of Bristol, UK)

Eberhard K.U. Gross (The Hebrew University of Jerusalem, Israel)

Emmanuel Fromager (Université de Strasbourg, France)

Carlos Benavides-Riveros (Max Planck Inst. Physics of Complex Systems, Dresden, Germany)

Matthieu Saubanère (Institut Charles Gerhardt Montpellier, France)

Pierre-Francois Loos (Centre National de la Recherche Scientifique, Toulouse, France)

Mauricio Rodríguez Mayorga (Vrije Universiteit Amsterdam, Netherlands)

Alexander Sokolov (Ohio State University, USA)

Stefano Di Sabatino (Lab. de Chimie et Physique Quantiques - IRSAMC, Toulouse, France)

Pina Romaniello (Université Paul Sabatier, Toulouse, France)

Nicholas Cox (CREOL, University of Central Florida, USA)

Geza Toth (Faculty of Science and Technology, UPV/EHU, Spain)

Róbert Trényi (Faculty of Science and Technology, UPV/EHU, Spain)

Kasia Pernal (Institute of Physics, Lodz University of Technology, Lodz, Poland)

II International Conference on Novel 2D Materials Explored via Scanning Probe Microscopy & Spectroscopy (2DSPM)

June 20-24, 2022
Miramar Palace, Donostia/San Sebastián
http://2dspm.dipc.org/

Organizing Committee
Miguel Moreno Ugeda (Ikerbasque, CFM-UPV/EHU, DIPC)
Iván Brihuega (UAM, Madrid)
Karmela Alonso (DIPC)

The possibility of engineering artificial materials from 2D materials with atomic precision and with "à la carte" properties is becoming a reality. This dynamic field gives rise to frequent notable advances in the field that need to be shared and assumed by the scientific community. This conference, therefore, aimed to be a meeting point of international reference for researchers in 2D materials, whose main working tools are SPM microscopy techniques, a community of great weight in the field. The 2DSPM conference aimed to promote interaction and the generation of common solutions between experimental and theoretical scientists in this field, creating a meeting space to share the latest advances in the development of experimental techniques, simulation methods and characterization of novel 2D materials.

Invited Speakers
Ali Yazdani (Princeton University, USA)
Abhay Pasupathy (Columbia University, USA)
Eva Andrei (Rutgers University, USA)
Andrei Bernevig (Princeton University / DIPC)
José Ignacio Pascual (CIC nanoGUNE, Spain)
Roland Wiesendanger (UHH, Germany)
Irina Grigorieva (Manchester University, UK)
Joseph Stroscio (NIST, USA)
Joaquín Fernández-Rossier (INL Braga, Portugal)
Vidya Madhavan (UIUC, USA)
Peter Liljeroth (Aalto University, Finland)
Roman Fasel (EMPA, Switzerland)
Ion Errea (UPV/EHU, Spain)
Arkady Krasheninnikov (HZDR, Germany)
Ernst Meyer (Basel University, Switzerland)
Tristan Cren (Sorbonne University, France)
Renard Vincent (CNRS Grenoble, France)
Aran García-Lekue (DIPC, Spain)
Sivan Refaeli-Abramson (Weizmann Institute, Israel)
Amadeo López de Parga (UAM, Spain)
Milan Allan (Leiden University, The Netherlands)
Pavel Jelinek (I. Physics, Czech Republic)

The Taming of Energy

July 4-6, 2022
Miramar Palace, Donostia/San Sebastián
https://www.uik.eus/en/activity/domesticacion-energia

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

Energy is often defined as the ability to do work, but its precise meaning depends on the context in which it is used. In the Summer Course "The Taming of Energy", organized in collaboration between the UPV/EHU Chair of Scientific Culture and DIPC, we analyzed the role of energy in very different scenarios and explained how it has defined the evolution of very different systems, either spontaneously or guided by human purpose.

The Course began with the presentation of the concept of energy in two contexts typical of physics: the universe and the quantum world. It continued with a brief review of energy transitions in human history, as well as a description of current scientific advances on the road to sustainability. On the second day, the energy flows that occur in living systems were presented. Last but not least, different stages of its industrial use were reviewed.

In short, the course consisted of a journey through the different ways in which living organisms and societies have made use of energy, for which they have had to "tame" it.

Invited Speakers
Violeta González Pérez (CIAF/UAM, Spain)
Ricardo Díez Muiño (DIPC/CFM, Spain)
Maria del Mar Rubio Varas (UPNA, Spain)
Sara Barja Martínez (CFM-UPV/EHU, Spain)
Nagore Ortiz Vitoriano (CIC Energigune, Spain)
Carlos Briones Llorente (CSIC, Spain)
Unai Ugalde Martínez (UPV/EHU, Spain)
Raquel Esteban Terradillos (UPV/EHU, Spain)
Miren Bego Urrutia Barandika (UPV/EHU, Spain)
Juan Ignacio Pérez Iglesias (UPV/EHU, Spain)
Ambrosio Liceaga Elizalde (UPNA, Spain)
Joaquín Sevilla Moróder (UPNA, Spain)
Teresa Valdés Solís (CSIC, Spain)
Noemí González Sabugal (Writer, Spain)

Novel Electronic Properties of Two-dimensional Materials

July 11-15, 2022
Miramar Palace, Donostia/San Sebastián
http://www.nep2dm.dipc.org

Organizing Committee
Francisco Guinea (IMDEA/DIPC)
Pablo Jarillo-Herrero (MIT)
Fernando de Juan (DIPC)
Frank Koppens (ICFO)

Since the discovery of superconductivity in rotated graphene bilayers by Pablo Jarillo-Herrero's group at MIT, the field of so-called moiré heterostructures has positioned itself as one of the most active in all of condensed matter physics. The field brings together experts from many long-standing fields such as superconductivity in correlated fermions, two-dimensional materials, and material topology, and has led to some of the most amazing discoveries of the last decade. The conference program was focused on bringing together the best theoretical and experimental experts in the field, with the idea of presenting the latest results in the field, discussing their implications and generating an exchange of ideas that lead to new discoveries. The conference more than met expectations, showing that the field maintains a growing interest and potential for the coming years.

Invited Speakers

Dimitry Basov (Columbia, USA)
Eun Ah Kim (Cornell University, USA)
Päivi Törmä (Aalto University, Finland)
Andrei Bernevig (Princeton, USA)
Atac Imamoglu (ETH Zurich, Switzerland)
Dimitry Efetov (Munich, Germany)
Hector Ochoa (DIPC/Columbia, Spain/USA)
Laura Classen (MPI-FKF, Stuttgart, Germany)
Alexey Berdyugin (Manchester University, UK)
Nick Bultinck (Oxford University, UK)
Jeanie Lau (Ohio State University, USA)
Xiaodong Xu (Washington University, USA)
Stevan Nadj-Perge (Caltech University, USA)
Daniel Parker (Harvard University, USA)
Jane (Jeong Min) Park (MIT, USA)
Mikito Koshino (Osaka University, Japan)
Leni Bascones (ICMM, Madrid, Spain)
Oleg Yazyev (EPFL, Switzeland)
Carmen Rubio-Verdú (Columbia, USA)
Pierre Pantaleon (IMDEA, Madrid, Spain)
Klaus Ensslin (ETH Zurich, Switzerland)
Yuval Oreg (Weizmann Institute of Science, Israel)
Jennifer Cano (Stony Brook University, USA)
Eli Zeldov (Weizmann Institute of Science, Israel)
Jeil Jung (University of Seoul, South Korea)
Cecile Repellin (CNRS Grenoble, France)

Quantum Designer Physics 2022 (QDP2022)

July 18-21, 2022
Miramar Palace, Donostia/San Sebastián
https://qdp2022.dipc.org/

Organizing Committee
Daniel Loss (University of Basel)
Paco Guinea (IMDEA Nanoscience, DIPC)
Andrés Arnau (UPV/EHU)
Vitaly Golovach (UPV/EHU, Ikerbasque)

The workshop aimed to highlight advances in material systems designed for studying the most intriguing physical phenomena at the nanoscale. These phenomena are related to spin, topology, and coherence, which make it possible for the materials to display quantum functionalities. While Condensed Matter Physics is rich in material systems in which almost any physics can be readily found and studied, with recent developments of quantum materials, it is possible to purposefully design material systems with a given physical phenomenon in mind. Thus, a 'toy model' which could be conceived to exhibit an interesting behavior can be implemented in quantum materials and be subsequently used for basic research and applications.

This workshop brought together the leading experts working on quantum materials and created a stimulating atmosphere for discussing physics on the marvelous sites of San Sebastian. We discussed recent progress in creating ordinary and topological quantum systems in different dimensions, as well as some of the most exotic quantum materials based on graphene and other low dimensional materials. We updated on the progress in spin-based quantum computing with an outlook into the prominent future of quantum technologies. The quest for Majorana bound states in hybrid superconducting systems and topological quantum computing and its problematics were also addressed. The workshop had all it is required to foster collaborations and inspire its attendants to tackle new problems with great ideas which make a difference for fundamental physics, lead to applications, and advance quantum technologies.

Invited Speakers

Silvano De Franceschi (CEA Grenoble and Univ. Grenoble Alpes, France)
Eugene Demler (ETH Zürich, Switzerland)
Klaus Ensslin (ETH Zürich, Switzerland)
Attila Geresdi (Chalmers University of Technology, Sweden)
Georgios Katsaros (Institute of Science and Technology Austria, Austria)
Alexander Khaetskii (Air Force Research Laboratory, Wright-Patterson AFB, USA)
Jelena Klinovaja (University of Basel, Switzerland)
Leo Kouwenhoven (QuTech and Kavli Institute, TU Delft, Netherlands)
Héctor Ochoa (DIPC, Spain)
Yuval Oreg (Weizmann Institute of Science, Israel)
Stuart Parkin (Max Planck Institute of Microstructure Physics, Germany)
Gloria Platero (ICMM-CSIC, Spain)
Marco Polini (Università di Pisa & Graphene Labs Genova, Italy)
Elsa Prada (ICMM-CSIC, Spain)
Yaroslav Tserkovnyak (University of California LA, USA)
Felix von Oppen (Freie Universität Berlin, Germany)
Amir Yacoby (Harvard University, USA)
Dominik Zumbühl (University of Basel, Switzerland)

NanoNeuro 2022

July 21, 2022
Live streamed
https://ntc.columbia.edu/nn22/

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

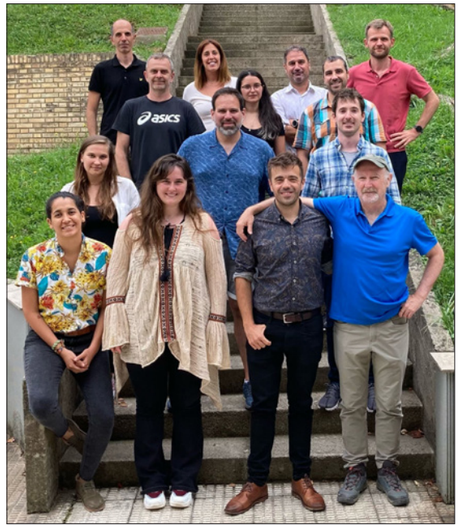
The conference aimed to help nucleate the emerging field of research at the intersection of Nanoscience and Neuroscience and provide a forum for experts from both areas to interact.

NanoNeuro2022 was an online conference, organized by the NeuroTechnology center at Columbia University and the Donostia International Physics Center (DIPC). The Conference was organized in thematic sessions with keynote and invited talks. This workshop was sponsored by the Tianqiao and Chrissy Chen Institute.

The conference achieved its scientific objectives and was followed by a total 1500 people, making it a great success of public as well.

Invited Speakers

Alice Ting (University of Stanford, USA)
Guillaume Baffou (CNRS, France)
Valentin Nageri (University of Bordeaux, France)
Sylvie Roke (EPFL, Switzerland)
Ozgur Shapiro (Caltech, USA)
Dirk Trauner (NYU, USA)
Viola Vogel (ETH Zürich, Switzerland)
Shimon Weiss (UCLA, USA)



MoLE Conference 2022

July 24-29, 2022
Tabakalera, Donostia/San Sebastián
http://moleconference2022.dipc.org

Organizing Committee
Aitzol García-Etxarri (DIPC)
Antonio García Martín (CSIC)
Cristina Sanz Fernandez (Multiverse Computing)
Edurne Sáenz Párraga (DIPC)
Jorge Olmos Trigo (DIPC)
Luis Froufe Pérez (Université de Fribourg)
Nuno de Sousa (DIPC)
Ricardo Diez Muiño (DIPC)
Pedro Miguel Echenique (DIPC)

The unexpected demise of Professor Juan José Sáenz, on March 22, 2020, left his beloved family and friends in shock all over the globe. Not by chance our friend Juanjo named his research group MoLE, standing for Moving of Light and Electrons, as a funny twist merging his passion for physics, colleagues, friends and family to whom, with no exception, Juanjo was known as Mole.

Following this spirit, MoLE conference 2022 was devoted to honouring his memory the way Mole would have liked: Appreciated colleagues and friends presenting and discussing their most recent advances, in both electronics and photonics. All that in the cosy atmosphere that only the city of Donostia, another Mole's passion, provides with.

The conference was a big success. It gathered over a hundred experts in materials science, scanning probe microscopy, and nanophotonics.

Invited Speakers
Diego Romero-Abujetas (Fribourg University, Switzerland)
Pedro Miguel Echenique (DIPC, Spain)
Javier Aizpurua (CFM-CSIC, Spain)
Andrés Arnau (CFM-UPV/EHU, Spain)
Emilio Artacho (University of Cambridge, UK)
Agustina Asenjo (ICMM, Spain)
Sara Barja (CFM-UPV/EHU, Spain)
Alvaro Blanco (CSIC, Spain)
Andrea Bragas (Universidad de Buenos Aires, Argentina)
Ivan Brihuega (UAM, Spain)
Remi Carminati (Institut Langevin, ESPCI, France)
Jaime Colchero (Universidad de Murcia, Spain)
José Costa-Kramer (Instituto de Micro y Nanotecnología, Spain)
Gabriel Cwillich (Department of Physics, Yeshiva University, USA)
Rafael Delgado-Buscalioni (IFIMAC, UAM, Spain)
Sofía Sanz (DIPC, Spain)
Jochen Feldmann (Ludwig-Maximilians-Universität, Germany)
Jorge M. García (Instituto de Micro y Nanotecnología, Spain)
Javier García de Abajo (Institut de Ciències Fotòniques, Spain)
Francisco José García Vidal (Condensed Matter Physics Center, UAM, Spain)
Ricardo García-García (ICMM, Spain)
Aran García-Lekue (DIPC, Spain)
Maria García-Parajo (Institut de Ciències Fotòniques, Spain)
Maia García-Vergniory (Max Planck Institute for Chemical Physics of Solids, Germany)
Jean-Jacques Geffret (Université Paris-Saclay, France)
Sylvain Gigan (Sorbonne Universite, France)
Juan Jose Gomez-Cadenas (DIPC, Spain)
Cristina Sanz-Fernández (Multiverse Computing, Spain)
Gabriel Gomila (Institut de Bioenginyeria de Catalunya, Spain)
Beatriz Hernández-Juárez (ICMM, Spain)
Rainer Hillenbrand (CIC nanoGUNE BRTA, Spain)
Hajime Ishihara (Osaka Prefecture University, Japan)
David Jimenez Jimenez (UAB, Spain)
Maria Kafesaki (University of Crete, Greece)
Daniel Kimura (Université Paris-Saclay, France)
Judith Langer (CIC biomaGUNE, Spain)
Luis Liz-Marzan (CIC biomaGUNE, Spain)

Cefe Lopez (ICMM, Spain)
Monica Luna (ICMM, Spain)
Stefan Maier (Imperial College London, London)
Onofrio Maragó (Istituto per i Processi Chimico-Fisici, Italy)
Manuel Marques (UAM, Spain)
Lluis Marsal (Rovira I Virgili University, Spain)
Luis Martin Moreno (Universidad de Zaragoza, Spain)
Jose Angel Martin-Gago (ICMM, Spain)
Javier Méndez (ICMM, Spain)
Gabriel Molina-Terriza (CFM-UPV/EHU, Spain)
Pablo Ordejon (T2 Catalan Institute of Nanoscience and Nanotechnology, Spain)
Roberto Otero (IMDEA-Nanoscience Center, Spain)
Ramón Paniagua (Institute of Materials Research and Engineering, Singapore)
Nacho Pascual (CIC nanoGUNE-BRTA, Spain)
Helmut Ritsch (Institut für Theoretische Physik, Universität Innsbruck, Austria)
Monika Ritsch-Marte (Institute of Biomedical Physics, Austria)
Stefan Roche (Institució Catalana de Recerca i Estudis Avançats, Spain)
Celia Rogero (CFM-CSIC, Spain)
Luis Rojas (Departamento de Física, CINVESTAV-IPN, México)
Halina Rubinsztein-Dunlop (The University of Queensland, Australia)
Jose Sanchez-Gil (CSIC, Spain)
Daniel Sanchez-Portal (CFM-CSIC, Spain)
Ricardo Sapienza (Imperial College London, UK)
Frank Scheffold (University of Fribourg, Switzerland)
Jose Soler (Condensed Matter Physics Center, Spain)
Jesus Ugalde (DIPC, Spain)
Niek Van Hulst (Institut de Ciències Fotòniques, Spain)
Silvia Vignolini (University of Cambridge, UK)
Giovanni Volpe (Gothenburg University, Sweden)
Miztli Yepez (Universidad Autónoma Metropolitana, México)
Rubén Esteban (CFM-CSIC, Spain)
Vladimiro Mujica (Arizona State University, USA)
Jon Lasa-Alonso (CSIC-UPV/EHU, Spain)
Antonio García-Martín (Instituto de Micro y Nanotecnología, Spain)
Jorge Olmos-Trigo (DIPC, Spain)
Aitzol García-Etxarri (DIPC, Spain)
Edurne Sáenz-Párraga (DIPC, Spain)

11th Conference on Broadband Dielectric Spectroscopy and its Applications (BDS2022)

September 4-9, 2022
Cámara de Comercio, Donostia/San Sebastián
http://bds2022.dipc.org/

Organizing Committee
Silvina Cerveny (CFM-CSIC)
Gustavo A. Schwartz (CFM-CSIC)
Daniele Cangialosi (CFM-CSIC)
Silvia Arrese-Igor (CFM-CSIC)

Broadband dielectric spectroscopy (BDS) is a powerful experimental technique permitting the investigation of the molecular dynamics of polar (and nonpolar) materials over a wide frequency range covering up to 16 decades at different temperatures and pressures. BDS finds a considerable number of applications in various fields of science and technology.

BDS2022 provided a platform to discuss the exciting new developments of broadband dielectric spectroscopy at both the academic and industrial levels. There were 90 talks (invited and orals) to discuss the latest results in the field. In addition, there were two sessions for young researchers in the first years of their Ph.D. These sessions helped to seed a new generation of working people on this technique. Finally, there was a session of the board of the International Dielectric Society in San Sebastian.

Invited Speakers
Karolina Adrjanowicz (University of Silesia, Poland)
Christiane Alba-Simionesco (Université Paris-Saclay, France)
Angel Alegria (CFM-UPV/EHU, Spain)
Thomas Blochowicz (Technical University of Darmstadt, Germany)
Simone Capaccioli (Università di Pisa, Italy)
Shinian Cheng (University of Silesia in Katowice, Poland)
Natalia Correia (Université de Lille, France)
Laurent Delbreilh (Université de Normandie, France)
Maria Madalena Dionísio (University of Lisbon, Portugal)
Tiberio Ezquerra (Instituto de Estructura de la Materia, IEM-CSIC, Spain)
George Floudas (University of Ioannina, Greece)
Koji Fukao (Ritsumeiken University, Japan)
Caroline Genix (University of Montpellier, France)
Martina Havenith (Ruhr University Bochum, Germany)
Tina Hecksher (Roskilde University, Denmark)
Paul Ben Ishai (Ariel University, Israel)
Friedrich Kremer (University of Leipzig, Germany)
Apostolos Kyritsis (National Technical University of Athens, Greece)
Roberto Macovez (Universitat Politècnica de Catalunya, Spain)
Simone Napolitano (Université libre de Bruxelles, Belgium)
Kristine Niss (Roskilde University, Denmark)
Aurora Nogales (Instituto de Estructura de la Materia, IEM-CSIC, Spain)
Ryusuke Nozaki (Hokkaido University, Japan)
Marian Paluch (University of Silesia in Katowice, Poland)
Ranko Richert (Arizona State University, USA)
Birte Riechers (Federal Institute for Materials Research and Testing, USA)
Ernst Rössler (Universität Bayreuth, Germany)
Andreas Schönhals (Bundesantalt für Materialforschung und -prüfung (BAM), Germany)
Clemens Sill (Goodyear Innovation Center Luxembourg, Luxembourg)
Michelina Soccio (University of Bologna, Italy)
Anatoli Serghei (Université Claude Bernard, Lyon, France)
Alexei Sokolov (University of Tennessee, USA)
Josep Tamarit (Universitat Politècnica de Catalunya, Spain)
Jan Swenson (Chalmers University of Technology, Sweden)
Michael Vogel (Technical University of Darmstadt, Germany)
William Hunter Woodward (The Dow Chemical Company, USA)
Michael Wübbenhorst (KU Leuven, Belgium)

Origin, Growth and Feedback of Black Holes in Dwarf Galaxies (dwarfbh2022)

September 12-16, 2022
Live streamed and in-person
Miramar Palace, Donostia/San Sebastián
http://dwarfbh2022.dipc.org/

Organizing Committee
Silvia Bonoli (DIPC)
Lucio Mayer (University of Zurich)
Mar Mezcua (Institute of Space Sciences, Barcelona)
Luis Ho (Kavli Institute for Astronomy and Astrophysics, Beijing)
Justin Read (University of Surrey)

The goal of the conference was to bring together the community interested in understanding the formation and evolution of massive black holes in dwarf galaxies.

During the conference we reviewed the current observational status concerning active black holes in dwarf galaxies, and discussed the prospects of new methods to identify them, including gravitational waves experiments, dynamical measurements and tidal disruption events. We reviewed and discussed theoretical models for the origin of black hole seeds, and how they might be a different population than that of supermassive black holes in normal galaxies. We also discussed models for the growth of massive black holes and their feedback onto the surrounding galaxies. We also reviewed the fundamental properties of dwarfs as predicted by hierarchical galaxy formation models in the LCDM framework, focusing on the interplay between galaxy and black hole growth modulated by feedback effects.

The meeting included the active participation of 90 scientists, approximately 60 attending in person and 30 remotely. On top of reviews from leading scientists in the field, the program included contributed talks and poster presentations, in large fraction from early career researchers. Every session also included time for discussions. Finally, we organized two round tables between early career researchers and two leading female scientists in the field.

Invited Speakers

Jillian Bellovary (City University of New York, USA)
Michelle Collins (Surrey University, UK)
Elena Gallo (University of Michigan, USA)
Jenny Greene (Princeton University, USA)
Paulina Lira (University of Chile, Chile)
Nadine Neumayer (Max Planck Institute for Astronomy, Germany)
Amy Reines (Montana State University, USA)
Elena Rossi (Leiden University, The Netherlands)
Anil Seth (University of Utah, USA)
Marta Volonteri (Institut d'Astrophysique de Paris, France)
Joe Silk (Institut d'Astrophysique de Paris, France)

Membrane Technologies for the Treatment and Recovery of Water Resources

October 10-11, 2022
Live streamed and in-person
Centro de Física de Materiales, Donostia/San Sebastián

Organizing Committee
Silvina Cerveny (CFM-CSIC)
Silvia Goyanes (Universidad de Buenos Aires and CONICET)
Jose Vega Baudrit (LANOTEC, Costa Rica)

We discussed different technologies to remediate water from pollutants (arsenic, pharmaceuticals, dies, and other heavy metals). Adsorption and phytoremediation were the two more cited methods to clean water. In addition, we discussed how these technologies can reach the market.

Invited Speakers

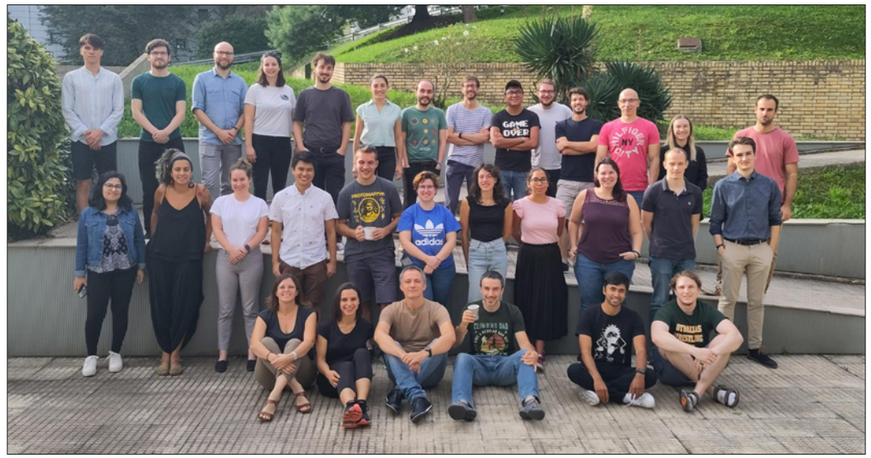
Silvia Goyanes (Universidad de Buenos Aires – CONICET, Argentina)
Silvina Cerveny (CFM, CSIC, Spain)
Elizabeth Agostini (Universidad Nacional de Río Cuarto, Argentina)
José Vega Baudrit (LANOTEC, Costa Rica)
Guillermo Grindlay (Universidad de Alicante, Spain)
Paola P. Pereira (Universidad Nacional de Río Cuarto, Argentina)
Lucas G. Sosa Alderete (Universidad Nacional de Río Cuarto, Argentina)
Nicolas Torasso (Universidad de Buenos Aires, Argentina)
David Picón (Universidad de Buenos Aires, Argentina)
Alicia Vergara-Rubio (Universidad Nacional de San Martín, Argentina)
Javier Martinez Sabando (MPC, Spain)
Francesco Coin (MPC, Spain)

Young Astronomers on Galactic Nuclei–2022 edition (YAGN2022)

January 8-10, 2022
Carlos Santamaría Centre, Donostia/San Sebastián
https://yagn2022.dipc.org/index.html

Organizing Committee
Silvia Bonoli (DIPC, San Sebastián)
Pedro Capelo (University of Zurich)
Massimo Dotti (University of Milano, Bicocca)

Young Astronomers on Galactic Nuclei (YAGN) is an annual series of informal meetings of PhD students and postdocs working on supermassive black holes and active galactic nuclei in general, with the aim of promoting exchanges of ideas and new collaborations among young scientists.



Invited Speakers
Anelise Audibert (Instituto de Astrofísica de Canarias, Spain)
Sara Cazzoli (Instituto de Astrofísica de Andalucía, Spain)
Laura Hermosa Munoz (Instituto de Astrofísica de Andalucía, Spain)
Romain Meyer (Max-Planck-Institut für Astronomie, Germany)
George Mountrichas (Instituto de Física de Cantabria, Spain)
Nathan Steinle (University of Birmingham, UK)

One Hundred Years of IUPAP. A Workshop

October 20-22, 2022
Cámara de Comercio, Donostia/San Sebastián
https://www.uik.eus/es/curso/one-hundred-years-iupap-workshop

Organizing Committee
Jaume Navarro (UPV/EHU, Ikerbasque)
Roberto Lalli (Max Planck Institute for the History of Science)

The workshop discussed pre-circulated papers on different aspects of the history of the International Union of Pure and Applied Physics (IUPAP). These will become the chapters of an edited volume to be published by Oxford University Press (already under contract) in 2023. The main themes of the papers related to institutional history, to the changing definitions of pure and applied physics, to the emerging topic of science as diplomacy, and to the role of international institutions as agents of science globalization.

Invited Speakers
Daniele Cozzoli (Pompeu Fabra University, Barcelona, Spain)
Connemara Doran (Harvard University, USA)
Danielle Fauque (Paris-Saclay University, France)
Robert Fox (Oxford University, UK)
Karl Grandin (The Royal Swedish Academy of Sciences, Stockholm, Sweden)
Barbara Hof (University of Zurich, Switzerland)
Danian Hu (City College, NY, USA)
Alexei Kojevnikov (University of British Columbia, Vancouver, Canada)
Jinyan Liu (Chinese Academy of Sciences, China)
Kenji Ito (Graduate University for Advanced Studies, Hayama, Japan)
Roberto Lalli (Max Planck Institute for the History of Science, Berlin, Germany)
Joseph D. Martin (Durham University, Durham, UK)
Gisela Mateos (Universidad Nacional Autónoma de México, Mexico)
Jaume Navarro (UPV/EHU, Ikerbasque, Spain)
Doubravka Olšáková (Academy of Sciences of the Czech Republic)
Pablo Ruiz de Olano (Max Planck Institute for the History of Science, Berlin, Germany)
Climerio da Silva Neto (Federal University of Bahia, Brazil)
Josep Simon (University of Valencia, Spain)
Brigitte van Tiggelen (Science History Institute, Paris, France)
Simone Turchetti (University of Manchester, UK)
Luciana Vieira Souza da Silva (University of São Paulo, Brazil)
Xiaodong Yin (Capital Normal University, Beijing, China)

Transborder QuantumChemPhys Lab Workshop 2022

December 13-14, 2022
Hotel Le Bayonne, Bayonne (France)
http://dipc.ehu.es/ws_presentacion.php?id=280

Organizing Committee
Pascal Larregaray (ISM, Université de Bordeaux, France)
Ricardo Díez Muiño (CFM, DIPC, Donostia/San Sebastián, Spain)

Theoretical Chemistry and Physics at the Quantum Scale (QuantumChemPhys) is a Transborder Joint Laboratory (LTC - Laboratoire Transfrontelier Conjoint, http://www.quantumchemphys.org) created by Université de Bordeaux (UBx), Universidad del País Vasco / Euskal Herriko Unibertsitatea (UPV/EHU), and Donostia International Physics Center (DIPC). The purpose of the QuantumChemPhys lab is to strengthen the scientific collaboration among researchers from Euskadi and Aquitaine through the creation of a transnational institution focusing on the theoretical aspects of chemistry and physics at the quantum scale, i.e. the quantitative description of the motion of electrons and nuclei (and their coupling) in solids, at gas-solid interfaces, as well as in the interaction with light. Such a challenge requires the developments of theoretical methods and numerical simulations within the framework of quantum/classical/semiclassical mechanics.

In this context, on December 13th-14th 2022, the QuantumChemPhys Lab organized a workshop in which recent activity on the topics of interest to the Lab were discussed. Forty scientists from the three institutions forming the QuantumChemPhys Lab gathered in Baiona. All PhD students developing their research project under the joint supervision of scientists in Donostia and Bordeaux had the opportunity to present their work in the workshop. Contributions from other junior researchers were scheduled as well. Possibilities of further collaboration among the institutions forming the Transborder Lab were explored. The workshop contributed to keep the cohesiveness of the QuantumChemPhys Lab, as well as to build and develop new lines of research.

Invited Speakers
Felana Adriambelaza (Université de Bordeaux, France)
Andrés Bejarano (DIPC, Spain)
Roberto Boto (DIPC, Spain)
Abel Carreras (DIPC, Spain)
Antonio Cebreiro (DIPC, Spain)
Angela Dellai (Université de Bordeaux, France)
Xabier Diaz de Cerio (DIPC, Spain)
Sophie Espert (Université de Bordeaux, France, CFM, Spain)
Oihana Galparsoro (UPV/EHU, Spain)
Asier Izu (DIPC, Spain)
Jean-Marc Leyssale (Université de Bordeaux, France)
Sara Lois (DIPC, Spain)
Carolina Martínez Strasser (DIPC, Spain)
Carmelo Naim (Université de Bordeaux, France, DIPC, Spain)
Minh Nguyen (DIPC, Spain)
Amael Obliger (Université de Bordeaux, France)
Norhan Omar (Université de Bordeaux, France)
Josianne Owona (Université de Bordeaux, France, DIPC, Spain)
Mario Piris (UPV/EHU, DIPC, Spain)
José Aarón Rodríguez Jiménez (DIPC, Spain)
Juan Carlos Roldao (U. Lund, Sweden, U. Bordeaux, France, DIPC, Spain)
Jorge Sánchez Dolado (CFM, Spain)
Claire Tonnelé (DIPC, Spain)

New Trends in Complex Quantum Systems Dynamics 2022

June 20-24, 2022
Carlos Santamaría Centre, Donostia/San Sebastián
https://www.uik.eus/en/activity/new-trends-complex-quantum-systems-dynamics-2022

Organizing Committee
Simone Montangero (Padova University)
Javier Prior (Murcia University)
Enrique Rico (UPV/EHU, Ikerbasque)

Local Committee
Miguel García Echevarria (UPV/EHU)
Iñigo Luis Egusquiza (UPV/EHU)
Gunar Schnell (UPV/EHU, Ikerbasque)

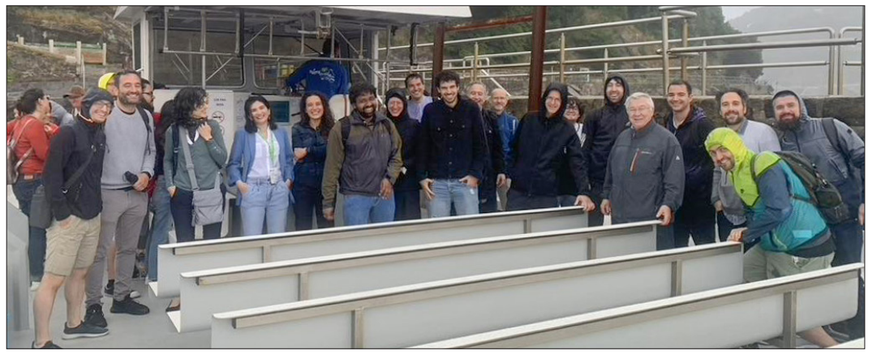
In our Quantum Science era where fault-tolerant quantum devices are still not available but Noisy Intermediate-Scale Quantum (NISQ) devices are accessible, quantum information tools to guide their development play a fundamental role. With the foreseen increasing complexity of available NISQ devices, their classical simulations - which drove their development until now - will soon fail to keep up. There is thus an urgent need for increasingly powerful diagnostic tools that can be applied to quantum devices even in the quantum advantage regime. At the center of the quantum-inspired algorithms lay tensor networks, one of the most powerful paradigms for simulating quantum many-body lattice systems, both in- and out-of-equilibrium, via a representation of the quantum state with tailored variational ansatz wave functions. The results of this workshop will be an essential tool to advance our understanding of dynamical and strong-correlation effects in quantum matter also beyond the NISQ era. Our activity is only possible thanks to a collaborative effort between theory and experiment, and an interdisciplinary approach leveraging the combined expertise of researchers from atomic, molecular, and optical (AMO) quantum technologies (QTs), and high-energy physics. This workshop brings together various key actors who will influence the future development of the leading QTs. The results shown in this workshop will have applications ranging from condensed matter physics over high-energy physics to quantum information theory, facilitating the design of new materials, and even more efficient chemical reactions.

This workshop showed highly collaborative advanced multidisciplinary science and innovative engineering project with the potential to initiate and foster new lines of quantum technologies:

- Quantum simulation and computation: the planned talks in the workshop will showed new ways to use existing quantum platforms and apply them to chemistry, condensed matter, and high-energy physics, among others.
- Quantum information science: the planned talks in the workshop will showed paradigmatic tools to analyse and study quantum systems for quantum information purposes.
- Quantum sensing: the planned talks in the workshop will showed paradigmatic tools to analyse and study magnetic field sensing with super resolution spectroscopy and single-molecule NMR.

The impacts of the workshop were:

- Develop a deeper fundamental and practical understanding of systems and protocols for manipulating and exploiting quantum information with the invited and contributed talks and the poster session.
- Identify new opportunities and applications to be fostered through quantum technologies, creating synergies among the most important researchers in the community.
- Enhance interdisciplinary in crossing traditional boundaries between disciplines to enlarge the community involved in tackling these new challenges, with this in-person activity.



Invited Speakers
Natalia Ares (Oxford University, UK)
Mari Carmen Bañuls (MPQ, MCQST, Germany)
Alejandro Bermudez (CSIC, Spain)
Rainer Blatt (Universitat Innsbruck, IQOQI, Alpine Quantum Technologies GmbH, Austria)
Giuseppe Clemente (DESY Zeuthen, Germany)
Marcello Dalmonte (SISSA, ICTP, Italy)
Zohreh Davoudi (University of Maryland, USA)
Gary Goldstein (Tufts University, USA)
Fedor Jelezko (Institute for Quantum Optics, Ulm University, Germany)
Zala Lenarčič (Jozef Stefan Institute, Slovenia)
Fernando Luis Vitalla (INMA, CSIC-Universidad de Zaragoza, Spain)
Maria Jose Martínez Pérez (INMA, CSIC-Universidad de Zaragoza, Spain)
Hannes Pichler (Universitat Innsbruck, IQOQI, Austria)
Martin Ringbauer (Institut fur Experimentalphysik, Universitat Innsbruck, Spain)
Sofia Vallecorsa (CERN, Switzerland)
Andreas Schäfer (Regensburg University, Germany)

International Conference on Science and Technology of Quantum Matter (QUANTUMatter 2022)

June 21-23, 2022

AXA Convention Center, Barcelona

https://www.quantumconf.eu/2022/about.php#about

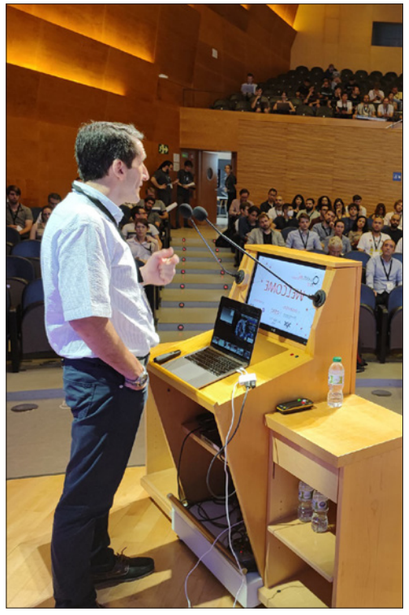
Organizing Committee

Antonio Correia (Phantoms Foundation)
Ricardo Díez Muiño (DIPC, CFM-CSIC)
Juan Jose Garcia-Ripoll (IFF-CSIC)
Pablo Ordejón (ICN2)
Jordi Arbiol (ICREA/ICN2, Spain)
Leticia Tarruell (ICFO, Spain)
Pol Forn-Díaz (IFAE, Spain)
Alba Cervera Lierta (Barcelona Supercomputing Center, Spain)
John Calsamiglia Costa (UAB, Spain)
Bruno Julia (Universidad de Barcelona, Spain)
Xavier Oriols (UAB, Spain)
Francesc Perez-Murano (CNM / CSIC, Spain)
Valerio Pruneri (ICFO, Spain)

The 2nd edition of the Quantum Matter International Conference – QUANTUMatter 2022 (Barcelona, Spain) – aimed at gathering the various communities engaged in the science and technologies of quantum information and quantum matter, to foster the incubation of new ideas and collaborations at the forefront of quantum technologies, emerging quantum materials and novel generations of quantum communication protocols, quantum sensing and quantum simulation.

Quantum Information and Quantum Matter are two components of revolutionary treatments of information, which are becoming cornerstones for discovering and implementing disruptive paradigms in quantum computation and quantum technologies.

They have huge potential to impact established industrial sectors or building novel industries, as evidenced by the race towards practical quantum computers, together with the use of quantum technologies for secure communication, sensing and simulations of the quantum world. Quantum Matter encompasses existing materials used in current quantum technologies and Qubits-based architectures design as well as the vast family of topological quantum materials in which symmetries, topology and entanglement are strongly intertwined, and give rise to spectacular phenomena such as exotic superconductivity, quantum spin liquids, quantum anomalous Hall effect, nontrivial fermionic excitations such as Majorana fermions or more exotic many-body states, ... The convergences and synergies between Q-information and Q-Matter are foundational and will keep flourishing in the next decade.



Invited Speakers

Charles Marcus (Niels Bohr Institute, Denmark)
Antonio Acín (ICREA/ICFO, Spain)
Tommaso Calarco (FZJ, Germany)
Francesca Ferlaino (LFU, IQOQI, Austria)
Jose Ignacio Latorre (CQT, Singapore)
Cristiane Morais Smith (UU, The Netherlands)
Neil Abroug (National Innovation Council, France)
Mete Atature (University of Cambridge, UK)
Leni Bascones (ICMM/CSIC, Spain)
Fernando Brandão (AWS, CALTECH, USA)
Jens Eisert (Freie Universität Berlin, Germany)
Alexandre Jaoui (ICFO, Spain)
Peter Leek (University of Oxford, UK)
Prineha Narang (Harvard University, USA)
Giulia Semeghini (Harvard University, USA)
Christoph Stampfer (RWTH, Germany)
Wolfgang Tittel (TU Delft, The Netherlands)
Sergio O. Valenzuela (ICREA/ICN2, Spain)
Maia G. Vergniory (MPI CPfS, Germany)
Andreas Wallraff (ETH Zurich, Switzerland)
Joel Wang (MIT, USA)
Marc Almendros (Keysight Technologies, Spain)
Sergio Boixo (Google, USA)
Niels Bultink (Qblox BV, The Netherlands)
Bob Coecke (Cambridge Quantum/Quantinuum, UK)
Yonatan Cohen (Quantum Machines, Israel)
Gianni Del Bimbo (Multiverse Computing, Spain)
Matthieu Desjardins (C12QE, France)
Oktay Goktas (Agnostiq, Canada)
David Hayes (Qantinuum, USA)
Loïc Henriet (Pasqal, France)
Michael Marthaler (HQS Quantum Simulations, Germany)
Carmen Palacios-Berraquero (Nu Quantum, UK)
Jelmer Renema (Quix Quantum, The Netherlands)
Heike Riel (IBM Research, Switzerland)
Niccolo Somaschi (Quandela, France)
Daniel Szombati (Qilimanjaro, Spain)

Physics in 2D Nanoarchitectonics (Colloquium within CMD29)

August 21-22, 2022
Manchester Central Convention Center, UK
https://iop.eventsair.com/cmd29/physics-in-2D-nanoarchitectonics

Organizing Committee
Aran García-Lekue (DIPC, Ikerbasque)
Aitor Mugarza (ICN2, ICREA)
César Moreno (University of Cantabria)
Rasmita Raval (University of Liverpool)

The "Physics in 2D Nanoarchitectonics" colloquium was held within the CMD29 Conference, the 29th edition of the biennial international scientific meetings coordinated by the Condensed Matter Division (CMD) of the European Physical Society and organized together with the Institute of Physics.

This colloquium was a follow-up of the one hosted by the GEFES2020CMD conference in 2020, and its aim was to bring together a leading group researchers, in addition to students, postdocs and other participants to share the latest contributions in the field of physics of functional 2D nanoarchitectures. The symposium covered all relevant theoretical and experimental aspects related to this class of materials, such as synthesis and characterization of their electrical, optical, thermal, and mechanical properties.

It is worth pointing out the high-quality and interdisciplinarity of the talks, both invited and contributed. This clearly raised the interest of the audience, as clearly manifested by the long and interesting question rounds. The main objective of the colloquium was thus successfully achieved, that is, to facilitate discussion about the latest advances and challenges, and to stimulate the generation of new ideas in the highly active field of nanostructured 2D materials.

Invited Speakers
Mads Brandbyge (DTU, Denmark)
Nuria Aliaga (ICREA-ICMAB, Barcelona, Spain)
Alexander Grüneis (University of Cologne, Germany)
Gabriela Borin Barin (EMPA, Switzerland)

On-Surface Synthesis (OSS22)

September 25-30, 2022
Hotel Eden Roc, Sant Feliu de Guixols, Girona (Spain)
http://oss22.dipc.org/

Organizing Committee
Dimas G. de Oteyza (CINN, DIPC)
Martina Corso (CFM, DIPC)
André Gourdon (CEMES)

On-surface synthesis unites the easy tunability of molecular materials and the promises of self-assembly as a revolutionary production method, with the sturdiness of covalently bonded structures. This most attractive combination is drawing the interest of a rapidly increasing number of researchers. Important efforts are being devoted to augment the available on-surface synthesis toolbox, to improve our understanding of the chemical reaction mechanisms, as well as to the synthesis and characterization of new molecular architectures of potential interest for diverse applications.

Because this approach bridges across the fields of chemistry, physics and materials science, the aim of this fourth edition of the "On-Surface Synthesis" international workshop was to bring together researchers working in this field from different perspectives, theory and experiment, as well as with chemical, physical and/or application-oriented viewpoints. This goal has been successfully achieved, bringing together most groups working in the field.

Invited Speakers
Jonas Björk (Linköping University, Sweden)
Sylvain Clair (Aix Mairseille University, France)
Mike Crommie (UC Berkeley, USA)
David Ecija (IMDEA Nanociencia, Spain)
Roman Fasel (EMPA, Switzerland)
Aran García-Lekue (DIPC, Spain)
Michael Gottfried (Phillips-Universität Marburg, Germany)
Leo Gross (IBM, Switzerland)
Pavel Jelinek (AV ČR, Czech Republic)
Shigeki Kawai (NIMS, Japan)
Peter Liljeroth (Aalto University, Finland)
Sabine Maier (FAU, Germany)
Francesca Moresco (TU Dresden, Germany)
Nacho Pascual (CIC nanoGUNE, Spain)
Alexander Sinitskii (UNL, USA)

5th Basque Quantum Science and Technology Workshop/ 1st IKUR QST Workshop

October 7, 2022

CIC nanoGUNE, Donostia/San Sebastián

http://dipc.ehu.es/giedke/eusqutech22.html

Organizing Committee

Enrique Rico (UPV/EHU, Ikerbasque)

Geza Giedke (DIPC, Ikerbasque)

The meeting continues a tradition started in 2015. It aims to bring together the growing community of researchers in the Basque Country working on or interested in quantum science and technology and related fields and to nurture and facilitate interaction, discussion, and collaboration. This year, we extended the geographic scope to invite speakers and participants form the University of Bordeaux as well.

With over 70 registered participants (including from Bordeaux and Tecnalia) and 29 submitted posters the workshop showcased the various approaches and questions related to quantum technologies that are addressed in the different groups and provided opportunity to initiate discussions about further collaborations, in particular across the border. Brief presentations of 8 relevant centers and initiatives in the "quantum" space clarified the institutional framework within which the workshop took place.

Invited Speakers

Iñigo Egusquiza (UPV/EHU, Spain)

Ruben Esteban (CFM-CSIC, Spain)

Aran García-Lekue (DIPC, Ikerbasque, Spain)

Ludovic Jaubert (Université de Bordeaux, France)

Vincent Ménoret (Université de Bordeaux, France)

Gonzalo Muga (UPV/EHU, Spain)

José Ignacio Pascual (CIC nanoGUNE, Ikerbasque, Spain)

Jean-Baptiste Trebbia (Université de Bordeaux, France)

Miguel Moreno Ugeda (DIPC, Ikerbasque, Spain)

8th International Doctoral Training Session: Frontiers of Condensed Matter

October 10-21, 2022
Les Houches, France
https://www.adum.fr/as/ed/page.pl?page=les_houches&site=phys

Organizing Committee
Sebastian Bergeret (DIPC, CFM-CSIC, Spain)
Julia Meyer (Université Grenoble Alpes, France)
Jörg Schmalian (Karlsruhe Institute of Technology, Germany)
Christian Schönenberger (University of Basel, Switzerland)
Gary Steele (TU Delft, The Netherlands)

Frontiers of Condensed Matter aims at offering final year Master students and junior PhD students a high-level training program in the general area of condensed matter physics. The session consists of lecture series on topics such as Quantum Transport, Topological Phases, Strongly Correlated Systems, and Quantum Information – complemented by more specialized pedagogical seminars on timely topics as well as poster sessions and discussion forums.

This was the 8th event in a series of doctoral training sessions organized since 2010. This session was organized jointly by the Physics Graduate School of Grenoble (France), the Casimir Research School of Delft-Leiden (Netherlands), the Donostia International Physics Center in San Sebastian (Spain), the Graduate School of Quantum Matter at the Karlsruhe Institute of Technology (Germany), and the Swiss Nanoscience Institute in Basel (Switzerland).

The session consisted of lecture series on the following topics:

- Quantum transport
- Superconductivity
- Topological phases
- Quantum information
- Circuit QED
- 2D materials

Complemented by more specialized pedagogical seminars on timely topics, poster sessions, and discussion forums.

Invited Speakers
Carlo Beenakker (Leiden University, The Netherlands)
Joerg Schmalian (Karlsruhe Institute of Technology, Germany)
Adolfo Grushin (CNRS, Grenoble, France)
Roman Orus (DIPC, San/Sebastián, Spain)
Benjamin Huard (ENS Lyon, France)
Dmitri Efetov (LMU Munich, Germany)
Gary Steele (TU Delft, The Netherlands)
Piet Brouwer (FU Berlin, Germany)
James Wootton (IBM Zurich, Switzerland)
Sophie Gueron (Université Paris-Sud, France)
Julia Meyer (U Grenoble, France)
Elke Scheer (U Konstanz, Germany)

Higher Education

Photo- and Electrocatalysis at the Atomic Scale (PECAS 2022)

June 20-23, 2022
Materials Physics Center (CFM) & Miramar Palace
http://pecas2022.dipc.org/

Organizing Committee
Sara Barja (Ikerbasque, CFM-UPV/EHU, DIPC)
Celia Rogero (CFM-CSIC-UPV/EHU, DIPC)
Ethan Crumlin (LBNL-ALS)
Martin Sterrer (University of Graz)

In collaboration with CAT&SCALE network:
Nuria López (ICIQ)
José Ramón Galán (ICIQ)
Sixto Gimenez (UJI)
Francisca López (ICMM)
David Écija (IMDEA Nanoscience)
Jordi Arbiol (ICN2)

PECAS 2022 was aimed at promoting interdisciplinary discussion of scientists in the material science and photoelectrochemistry fields in addition to presentation of new results, ideas and methods to understand the catalyst-electrolyte interface at an atomic level.

Introductory lectures -surface science, electrochemistry and theoretical methods- were specially addressed (2 days school) to introduce master and graduate students from Chemistry and/or Physics in each topic covered in PECAS2022. After two days of lectures and school-oriented event, PECAS2022 will allocate 2 days of workshop event, with invited seminars delivered at the postgraduate level in the fields of surface science and electrochemistry. In addition to the school lectures and invited talks, the scientific program was completed with 25 contributed orals.

Invited Speakers
Beatriz Roldán Cuenya (FHI, Germany)
Miquel Salmerón (LBNL, USA)
Jörg Libuda (FAU, Germany)
María Escudero-Escribano (KU, Denmark)
Sophia Haussener (EPFL, Switzerland)
Gareth Parkinson (TUwien, Austria)
Kelsey A. Stoerzinger (Oregon State University, USA)
Sixto Giménez (Universidad Jaume I, Spain)
Roberto Otero (UAM, Spain)
Barbara Lechner (TUM, Germany)
Ifan Stephens (Imperial College London, England)
Talat Rahman (University of Central Florida, USA)

Topological Matter School 2022 (TMS22)

August 22-26, 2022
Miramar Palace, Donostia/San Sebastián
http://tms.dipc.org/

Organizing Committee
Maia G. Vergniory (DIPC, MPI CPfS)
Reyes Calvo (Universidad de Alicante)
Santiago Blanco-Canosa (DIPC, Ikerbasque)
Fernando de Juan (DIPC, Ikerbasque)
Adolfo Grushin (Institut NEEL – CNRS)
Alexander Altland (University of Cologne)
Frank Pollmann (Technical University of Munich)

In 2022 edition we focused in understanding and exploiting the robustness of topological superconductivity and the unique quantum mechanical properties of strongly entangled particles is a thriving avenue to develop new quantum technologies. The first ideas and platforms, notably Majorana zero modes at the edges of one-dimensional topological superconductors, have led to a richer landscape of systems that include unconventional superconductors, spin-liquids, fractional quantum Hall states, as well as the simulation of many-body ground states in quantum computers. A hands-on session on quantum matter and AI with emphasis on quantum computing was also delivered. This new edition was devoted to pedagogically present the main recent developments in the field in order to prepare future generations to uncover the true potential of these developments.

Invited Speakers
Roser Valentí (Goethe-Universität, Germany)
Pedram Roushan (Google Inc, Santa Barbara, USA)
Charles Marcus (Niels Bohr Institute, Denmark)
Vidya Madhavan (UIUC, USA)
Eliska Greplova (TU-Deflt, The Netherlands)
Lucile Savary (CNRS, France)
Adam Smith (University of Nottingham, UK)
Jason Alicea (Caltech, USA)
Charlie Kane (University of Pennsylvania, USA)
Bella Lake (Helmholtz Zentrum Berlin, Germany)
Claudia Felser (MPG, Dresden, Germany)
Ady Stern (Weizmann Institute of Science, Israel)
Andrei Bernevig (Princeton University, USA)

Nanotechnology Meets Quantum Information (NanoQI'22)

August 30-September 2, 2022
Miramar Palace, Donostia/San Sebastián
http://nanoqi.dipc.org

Organizing Committee
Géza Giedke (DIPC, Ikerbasque)
Alejandro Gonzalez Tudela (IFF CSIC, Madrid)
Pascale Senellart (University Paris Saclay)
Juan Ignacio Cirac (MPI for Quantum Optics, Garching)
Atac Imamoglu (ETH Zurich)

The aim of the School was to provide an introduction to the basics, aims, methods, and recent advances in quantum information theory and solid-state-based quantum technologies and to highlight especially the benefits and challenges of coherent quantum physics and control of nanoscopic systems. Additionally, we aimed to provide a forum where young researchers can learn from recognized leaders in the field, meet and connect to colleagues and present their own research.

We believe that these aims were achieved thanks to 8 thorough and instructive lectures covering a wide variety of potential qubit implementations (from single atoms on surface through defect centers, quantum dots to majorana modes and superconducting circuits), followed by active discussions, and an intensive poster session (with over 25 posters), which provided plenty of time for the almost 80 students (mostly PhD students and some young postdocs) to interact.

Invited Speakers
Markus Aspelmeyer (Universität Wien, Austria)
Carlo Beenakker (Universiteit Leiden, The Netherlands)
Juan José García Ripoll (IFF CSIC Madrid, Spain)
Andreas Heinrich (QNS, Ewha Womans University, Seoul, South Korea)
Jason Petta (Princeton University, Princeton, NJ, USA)
Pascale Senellart (CNRS-C2N and Université Paris-Saclay, France)
Peter Rabl (Technische Universität Wien, Austria)
Jelena Vuckovic (Stanford University, CA, USA)

An Introduction to Time—Dependent Density Functional Theory

October 6-November 11, 2022
DIPC, Donostia/San Sebastián
http://dipc-courses.dipc.org/an-introduction-to-time-dependent-density-functional-theory

Eloy Ramos-Córdoba (UPV/EHU)
David Casanova (DIPC, Ikerbasque)
José M. Mercero (DIPC, UPV/EHU)
Jesús Ugalde (DIPC, UPV/EHU)
Eduard Matito (DIPC, Ikerbasque)

During 2022, there was a DIPC course devoted to time-dependent Density Functional Theory (TDDFT), a revolutionary technique involving theoretical chemistry and condensed-matter physics. The course was given by the important chemistry community at DIPC and the University of the Basque Country.

The course was 30 hours of theory and practical applications. It was a big success, surpassing 60 attendees in average, with interested researchers directly involved in the field, as well as other researchers looking for an efficient introduction into a complex and powerful technique.

The course consisted 15 sessions, where instructors gave a complete account of the theory allowing all interested researchers in the technique to become proficient and actualized in the different aspects and computational tools regarding TDDFT:

Review of ground-state density functional theory (E. Matito)
- Hohenberg & Kohn Theorem.
- Kohn-Sham DFT.
- Exact properties of density functionals.
- Density functional approximations: the Jacob's ladder.
- Functional derivatives.
- Density and density matrices.

Introduction to time-dependent phenomena (E. Matito)

The basic Formalism of TDDFT (E. Ramos-Cordoba)
- Fundamental existence theorems.
- The time-dependent Kohn-Sham equation.
- The adiabatic approximation.
- Numerical time propagation (Hand-on JM. Mercero)

Properties of the time-dependent xc potential (J. Ugalde)
- The universal functional and some exact conditions.
- Galilean invariance and the harmonic potential theorem.
- Memory, causality and initial-state dependency.
- Time-dependent variational principles.
- Energy discontinuities.

Linear-response TDDFT (J. Ugalde)
- General linear-response framework.
- Linear density response in TDDFT.
- The Casida equation.
- Tamm-Dancoff approximation.
- Time-dependent Hartree-Fock theory.

The frequency-dependent xc kernel (E. Ramos-Cordoba)
- Exact properties and approximations.
- The xc kernels of the homogeneous electron liquid.

Applications to atomic and molecular systems (D. Casanova)
- Excitation energies of small systems.
- Molecular excited-state properties with TDDFT.
- Double excitations.
- Charge-transfer excitations.
- The Sternheimer equation.
- Optical spectra via time propagation schemes.
- Generalized KS schemes for excited states.

Long-range correlations and dispersion interactions (E. Matito)
- The adiabatic-connection fluctuation-dissipation theorem.
- Van der Waals interactions.

Introduction to Artificial Intelligence in Basic Sciences

September 19-November 11, 2022
DIPC, Donostia/San Sebastián
http://dipc-courses.dipc.org/introduction-to-artificial-intelligence-in-basic-sciences

Luis A. Montero-Cabrera (University of La Habana, Cuba)

A not-less-important second course was the introduction to Artificial Intelligence in Basic Sciences, a timely and quickly evolving topic that is going to become a major subject of scientific curricula.

The course allowed attendants to become familiar with the essentials of artificial intelligence nature and methods in order to facilitate their understanding of procedures and current results. It also pursued to provide the necessary background for developing their own applications with available tools. Especial emphasis was made on machine learning techniques for treating databases, including the so-called "big data" referring to data sets that are too large or complex to be dealt with by traditional data-processing application software. It was intended for scientists familiar with basic computational sciences and advanced undergraduate students in Chemistry, Physics, Biology, Pharmacy and Biochemistry.

The course consisted in 3 sessions on basic theory, and 4 additional sessions to deal with relevant examples and applications:

- Information and systems.
- Computer systems.
- Boolean algebra.
- Intelligence.
- Artificial Intelligence.
- Intelligent agents.
- Percept sequence, performance measure, rational agents, task environments.
- Learning agents.
- Agent architecture and programing.
- Expert systems.
- Machine learning.
- Machine learning applications.
- Modeling, classification, regression, clustering.
- Data mining.
- Bayes theorem and applications.
- Bayesian networks.
- Naïve Bayes.
- Learning by Bayesian networks.
- Creating and teaching a machine.
- Machine learning paradigms: supervised, unsupervised and reinforced learning.
- Machine learning algorithms.
- Genetic algorithms as optimization processes.
- Artificial neural networks and "deep" learning.
- Machine learning applications.
- Data representations. "Inverse" machine learning.
- Some current relevant applications in science and shortcomings.
- Computational tools available.

Transferable Skills Courses

Equipping researchers with skills beyond the purely scientific is a challenge that institutions are beginning to take up in the framework of what is known as the "transferable skills" education programs. DIPC and CFM jointly run a full program covering issues like stress management, media training or transformative leaderships. 111 researchers joined these courses in 2022.

Emotional Intelligence at Work

November 30-December 1, 2022
CFM Auditorium, Donostia/San Sebastián

Sofia Facal
Skills for Science and Industry

Our social skills and emotional intelligence competencies are enriching factors in the workplace and our daily life. However, despite their importance, most individuals are not aware of these tools and how to develop them. This training was focused on the fundamentals of emotional intelligence and the understanding of how it plays a role in our interpersonal relationships at work. We applied effective methods to enrich ourselves and the diverse world of academia.

The content of the workshop included:

- The basics of Emotional Intelligence.
- Empathy and social skills: proficiency in managing relationships and building network.
- Building Emotional Intelligence of Groups.
- Emotional Intelligence and Diversity model: your cultural software.
- The art of influence.
- Collaboration and handling conflicts in the workplace.

Scientific Writing Basics

April 4-6, 2022
DIPC, Donostia/San Sebastián

Sofia Facal
Skills for Science and Industry

The ability to present scientific findings and information in a written format is an essential skill for everyone that wishes to pursue a career in science. Unlike other types of writing, scientific writing follows a specific format and style.

This workshop on scientific writing skills provided an outline of this format for a research paper, shines light on the publication and peer review process and gives basic tips for communicating complex topics in a logical, clear and understandable way.

The content of the workshop included:

- Scientific authorship and good scientific practice.
- Scientific journals and the peer review system.
- Scientific Paper Structure: objective, key content and length of the sections.
- Find your story: Development of the central idea.
- How to choose and organize the content.
- Handling raw data in publications.
- Images and graphics.
- The logical flow: Coherence and Cohesion.
- Do's and Don'ts of paper writing.

Creativity—Murakami Method

June 1-22, 2022
DIPC, Donostia/San Sebastián

Juan Luis Suárez
Director of CulturePlex Lab, Western University, Canada

The different elements of the Murakami Method were studied in the light of similar ideas contributed by scientists (Poincaré), mathematicians (Whitehead), writers (Poe, Proust, Trollope), artists (Doris Salcedo, Theaster Gates), musicians (Seiji Ozawa), and chefs (Adriá, Aduriz). The sessions were organized around the following themes: illuminations. training, craftsmanship and originality.

Mental Health Issues and the Ethics of Care in Research Intensive Institutions

May 24, 2022
DIPC, Donostia/San Sebastián

Erin Huner
Director of Culture & Inclusion, Ivey Business School, Canada

Why the growth of mental health issues in universities and research-intensive institutions? What is the ethics of care, that we need to collectively re-imagine when we think about student flourishing, academic success and equity and inclusion within our curricular and co-curricular learning environments? How might we re-imagine the ways in which the design of our learning spaces impacts student sense of wellbeing and belonging?

Dr. Erin Huner, Director of Culture & Inclusion, at the Ivey Business School, discussed approaches to designing curricular and co-curricular learning opportunities for students that center equity, inclusion and well-being, as a means of increasing student success and sense of belonging within the post-secondary landscape.

Theses

Design and topological characterization of 2D photonic.
María Blanco De Paz
27/01/2022
Supervisors: Aitzol García-Etxarri and Dario Bercioux

Título: Collective electronic and magnetic states in two-dimensional transition metal dichalcogenides.
Paul Dreher
25/03/2022
Supervisor: Miguel Moreno Ugeda

Computational studies on photophysical properties of molecular aggregates.
Olatz Uranga Barandiaran
25/03/2022
Supervisor: David Casanova Casas

The high-redshift formation and evolution of Super-Massive Black Holes
through semi-analytic models and photometric data.
Daniele Spinoso
30/03/2022
Supervisor: Silvia Bonoli

Thermoresponsive nano systems based on gold nanoparticles.
Joscha Kruse
15/07/2022
Supervisor: Marek Grzelczak

Insights into the efficient quantum chemical simulations of nonlinear optical properties.
Sebastian Sitkiewicz
22/07/2022
Supervisors: Eduard Matito Gras and Josep María Luís Luís

Ab initio many-body perturbation theory to study molecular systems: from implementation to applications.
Masoud Mansouri
04/10/2022
Supervisors: Daniel Sánchez Portal and Peter Koval

Pi-magnetism and quantum transport in grapheme-based nanostructures.
Sofía Sanz Whul
21/10/2022
Supervisor: Thomas Frederiksen

Theoretical study of excited triplet states of aromatic molecules for optoelectronic applications.
María Zubiría Ulacia
28/10/2022
Supervisors: David Casanova Casas and Jon Mattin Matxain Beraza

Quantum many-body effects in the optoelectronic response of plasmonic nanostructures
and their coupling to quantum emitters.
Antton Babaze Aizpurua
04/11/2022
Supervisors: Rubén Esteban Llorente and Javier Aizpurua Iriazabal

Design and chemical synthesis of fluorescent bicolor indicators for the detection
of neutrinoless double Beta decay of 136Xe.
Borja Aparicio Gil
21/11/2022
Supervisors: Iván Rivilla de la Cruz and Fernando P. Cossío Mora

Determination of nonlinear optical properties with quantum chemistry:
from benchmarks to experimental systems.
Carmelo Naim
02/12/2022
Supervisors: Eduard Matito Gras and Frédéric Castet

Computer simulations of intrinsically disordered proteins in the hypoxic response.
Irene Ruíz Ortíz
19/12/2022
Supervisors: David de Sancho Sánchez and Raúl Pérez Jiménez

UPV/EHU Research Master in Nanoscience

DIPC, along with CIC nanoGUNE, collaborates in the official Master in Nanoscience program organized by the University of the Basque Country (UPV/EHU) Department of Polymers and Advanced Materials: Physics, Chemistry and Technology and the Materials Physics Center (CFM-CSIC-UPV/EHU). The Master in Nanoscience has been offered since 2007 and presently more 170 students have obtained their Master's degree. 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: http://ehu.eus/en/web/master/master-nanoscience

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