

### ON THE COVER ADDING ROCKS TO THE SOUP

The elegant model of the early Earth designed by Miller-Urey demonstrated that applying lightning to a primitive reducing atmosphere and an alkaline sea could create a primordial soup containing the molecular building blocks of life. However, they overlooked the importance of minerals. We now understand that the experiment succeeds due to the role of silica and silicate minerals. These rocks also promote the formation of a solid organic film that self-organizes into protocells (seen in the image), thus recreating a chemical Hadean Protoworld capable of evolving towards greater chemical complexity and ultimately to primeval biochemistry. This discovery also has significant implications for detecting primitive life on Earth and elsewhere.

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DIPC ACTIVITY REPORT

uilding Connections	4
oard of Partners	7
esearch Activity at a Glance	8
IPC Supercomputing Center	10
cience Communication	12
quality at DIPC	28
cientific Highlights	33
ublications	73
IPC Community	124
esearchers	
isiting Researchers	
dministration and Services	170
eminars	
olloquia	
/orkshops	
ligher Education	219

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In today's rapidly evolving world, we navigate a complex global landscape. Geopolitical tensions have intensified and the international exchange of goods, ideas, and people seems increasingly threatened by mistrust and fragmentation. There remain however some powerful forces that continue to connect us. One of them is science, which is based on openness, collaboration, trust, and the free movement of ideas and people across cultures and continents. At DIPC, we are proud to be a part of this tradition.

Our research activity is international and interdisciplinary. Scientists from a wide variety of backgrounds work side by side, building connections that transcend borders. We believe that collective efforts are key to advancing knowledge. The great scientific challenges of our time-whether in quantum technologies, artificial intelligence, or fundamental physics-can only be addressed through global cooperation.

This vision of continuous collaboration and interconnectedness is mirrored by our own growth as an institution. The year 2024 has brought with it a defining development: the ongoing construction of a new building for DIPC, funded by the Department of Science, Universities and Innovation of the Basque Government. More than just a structural expansion, this project reflects the momentum that DIPC has gained in recent years—scientifically, intellectually, and socially. With more than 6,000 square meters of additional space and designed to host offices, experimental laboratories, and communal areas, the new facility will allow us to attract new talent, foster deeper collaboration, and embark on ambitious new research projects.

The new building will support and amplify our scientific core, now organized around four main thematic areas: QUANTUM, NANO, LIFE, and COSMOS. These areas encompass a dynamic research activity, which benefit from close partnerships with both local and international institutions. They reflect DIPC's commitment to science as a basis for long-term social and economic progress.

Beyond research, DIPC embraces the responsibility to be a cultural agent that engages with society. We want to contribute to a culture that values knowledge, creativity, and critical thinking. We believe that scientific culture is a cornerstone of a more open and tolerant society. In times of uncertainty and conflict, this mission becomes all the more urgent. Our outreach program, conceived with this very purpose, stands as one of the flagships of DIPC's activity. It reflects our belief in the transformative power of science within society.

None of this would be possible without the trust and support of our Board of Partners, which brings together public institutions and private organizations committed to the advancement of science. The meeting of the Board in December presided over by the new President of the Basque Government, Imanol Pradales, was a moment of recognition for DIPC's achievements. On this



Ricardo Díez Muiño, Director and Pedro Miguel Echenique, President

occasion, IBM officially joined the Board of Partners, further strengthening the ecosystem that sustains and drives our research forward. During the meeting, President Pradales remarked the importance of the Board's support in light of the center's growing size and impact and invited to all Partners to nurture the center's activity with a renewed ambition.

Last but not least, let us mention that the achievements of DIPC are the result of the exceptional efforts of our scientific, technical, and administrative staff. Their work is the driving force behind every achievement and every project of DIPC.

In a world of growing walls, science builds bridges. In a time of fragmentation, science offers connection. This belief guides our work at DIPC and inspires our vision for the years to come. This vision of continuous collaboration and interconnectedness is mirrored by our own growth as an institution.

Donostia International Physics Center (DIPC) is a research center opened in the year 2000. DIPC's mission is to carry out 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 entities (currently Kutxa Fundazioa. CAF, Telefónica, Fundación EDP and IBM) 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.

# Board of Partners

Pedro Miguel Echenique Landiribar President Juan Colmenero de León Vice President Ricardo Díez Muiño Director Alberto López Basaguren Secretary



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Horacio Morell Gálvez General Manager for Spain, Portugal, Greece and Israel (as of December 2024)









2000

KUTXA FUNDA ZIOA







TRM

IBM

# Research Activity at a Glance

The scientific production and impact of DIPC has grown year after year. In 2024, the center's scientific production set a record with **547 articles published**. But most important is the remarkable increase in the number of citations received by DIPC publications. Since 2000, DIPC has published a total of **6,350 ISI articles** and has received more than **262,200 citations**.



Source Web of Science Core Collection (all years and all indexes, 24/04/2025)



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, whereas international Workshops highlight specific subjects of interest. There are also DIPC Schools and Courses, especially aimed at young researchers and focused on learning particular skills. As well as DIPC Colloquia, which are colloquium-style lectures by outstanding speakers covering all areas of natural sciences. To reach a larger audience most of the programmed activities 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 Ikerbasque, 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

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 2024, the Center operates several supercomputers covering a wide range of computational needs. Its flagship system is the HYPERION supercomputer, inaugurated in February with the attendance of the Minister of Education of the Basque Government, Jokin Bildarratz.

HYPERION is a cluster featuring Xeon nodes, ranging from small nodes with 48 cores and 96 GB of RAM to large shared-memory nodes with 64 cores and 2 TB of RAM under a single operating system image. The supercomputing infrastructure includes 72 NVIDIA Tesla A100 GPUs, which are particularly suited for training large AI models. With over 16,000 cores and 200 TB of RAM, it ranks among the most powerful supercomputers in Spain. The construction of HYPERION was part of the overall strategy of the Basque Government to provide the scientific community with the necessary tools and infrastructures to carry out its work, in alignment with the strategic areas identified by the IKUR Strategy.



More than 600 researchers from DIPC and other research centers of the Basque Country such as UPV/EHU, Ikerbasque, the BERC centers, Achucarro, BC3, BCBL, BCAM, CFM/MPC, Biofisika, and BCMaterials, as well as, BioGipuzkoa, CIC BiomaGUNE, CIC NanoGUNE, Tecnalia, ESS Bilbao, Tecnun, Biobizkaia, Neiker, Orai, CIC BioGUNE, Deusto University, CIC EnergiGUNE, HiTZ Center, CEIT, Orai-Elhuyar, Vicomtech, BioAraba, AZTI, Aranzadi or Polymat used this computational infrastructure in 2024.



The Supercomputing Center team and DIPC's President and Director, along with the Minister of Education of the Basque Government Jokin Bildarratz, Deputy Minister of Universities and Research Adolfo Morais, and Director of Research Amaia Esquisabel during a visit to HYPERION supercomputer at DIPC.

# TOTAL CAPACITY Image: RAM Image: Scratch Disks Image: Home Directories Image: RAM Image: Scratch Disks Image: Home Directories Image: RAM Image: Scratch Disks Image: Scratch Disks Image: Home Directories Image: RAM Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: RAM Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: RAM Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: RAM Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: RAM Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: RAM Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: RAM Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: RAM Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: Scratch Disks Image: RAM Image: Scratch Disks

# Science Communication

2024 was a year of consolidation and further expansion of DIPC's science outreach program. One of the most iconic activities, Cinema and Science, attracted a record number of people in several cities, surpassing the 5,000 mark for the number of participants for the second year in a row. Emakumeak Zientzian, a celebration of the International Day of Girls and Women in Science was even more popular, with 13,500 people taking part in the numerous activities organized by 32 scientific and technological institutions in the Basque Country. In total, DIPC organized more than 160 activities throughout the year and reached over 38,000 people. This growing public interest encourages us to continue working to bring scientific knowledge closer to society.



Emakumeak Zientzian opening ceremony at the Intxaurrondo Cultural Center in Donostia/San Sebastián.

### EMAKUMEAK ZIENTZIAN

### 08-16/02/2024

The eighth edition of Emakumeak Zientzian brought together 32 science and technology institutions from the Basque Country to celebrate the International Day of Girls and Women in Science, which takes place on February 11th.

The following activities were organized or had direct involvement of DIPC: 08/02/2024 Intxaurrondo Cultural Center Donostia/San Sebastián Opening ceremony with all the volunteers 09/02/2024 Virtual tour of DIPC and CFM centers with our female scientists Schools 09/02/2024 Victoria Eugenia Club Aretoa, Donostia/San Sebastián 16/02/2024 Bidebarrieta Library, Bilbao Women scientists of yesterday and today Public lectures General public 08/02/2024 Artium Museum, Vitoria-Gasteiz 09/02/2024 Tabakalera, Donostia/San Sebastián 10/02/2024 Bizkaia Hall (UPV/EHU), Bilbao 13/02/2024 Golem Baiona Cinema, Pamplona Within Cinema and Science "Bombshell. The Hedy Lamarr Story" Screening presented by: Physicist Maia Garcia-Vergniory DIPC, Max Planck Institute for Chemical Physics of Solids Telecommunications Engineer Ane Insausti Provincial Council of Gipuzkoa, Mubil Fundazioa Computer Engineer Mari Luz Guenaga Deusto University General public For more information visit

Over the years, this collaborative project has spread throughout the Basque Country. In 2024, sixty activities were organized, 3 exhibitions, a video competition and a program of visits by female scientists to educational centers. In addition, a campaign under the slogan 'Living beyond science' was carried out on social networks to promote the reconciliation of a scientific career with a full life The main objectives of Emakumeak Zientzian are to increase the visibility of women in science, to challenge gender stereotypes associated with scientific and technical fields, and to encourage girls and young women to pursue careers in science. A record number of 13,558 people took part in the various activities in 2024. In total, it is estimated that 30,000 people have been reached directly in the eight editions, demonstrating the attractiveness and social impact of Emakumeak Zientzian. This success is mainly due to the enthusiasm and determination of hundreds of volunteer scientists (more than 300 in 2024) who participate in the project, but also to the institutions that have supported it. In 2024, the collaboration agreements reached with Fomento San Sebastián, the Provincial Council of Gipuzkoa, the Provincial Council of Bizkaia and BRTA were maintained, and new sponsors such as Ikerbasque and the companies SALTO and Casio joined the project. Other entities such as Donostia Kultura and Emakunde also collaborated through coprogramming or the allocation of spaces.

https://emakumeakzientzian.eus

	EMAKU	2024 Otsailak 8-16 Febrero		٢
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### CINEMA AND SCIENCE

The seventh Cinema and Science festival, organized jointly by DIPC, the Basque Film Archive, and the San Sebastián International Film Festival, took place from January to March. Ten films were presented by scientists in five cities, in the venues of our collaborators: Tabakalera (Donostia/San Sebastián), Bizkaia Aretoa of UPV/EHU (Bilbao), in lieu of the Bilbao Fine Arts Museum during the course of its expansion works, Artium (Vitoria-Gasteiz), Cines Golem (Pamplona) and Cinéma Le Sélect (Saint Jean de Luz, France).

This year's theme was the dilemmas and struggles of the scientific community, always aware of the historical moments that affect it. In total, more than 5,641 people attended the 47 programmed sessions.

### **General Sessions**

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

Oppenheimer (Christopher Nolan, 2023)\*/\*\* (1) 11/01/2024 (2) 11/01/2024 (3) 13/01/2024 (4) 16/01/2024 (5) 22/03/2024 Physicist Arantzazu Garcia-Lekue, DIPC, Ikerbasque Physicist Pedro Miguel Echenique, UPV/EHU, DIPC Physicochemist Didier Roux, Membre de l'Académie des Sciences et des Technologies

Semmelweis (André De Toth, 1940)\* (1) 18/01/2024 (2) 22/03/2024 (3) 20/01/2024 (4) 23/01/2024 (5) 15/01/2024 Physician Miguel Angel Goenaga, Hospital Universitario Donostia, OSI Donostialdea Microbiologist Ignacio Lopez Goñi, Universidad de Navarra, UNAV Historian Joxean Fernández, Basque Film Archive

 Out of Africa (Sydney Pollack, 1985)\*/\*\*

 (1) 25/01/2024
 (2) 26/01/2024
 (3) 27/01/2024

 (4) 30/01/2024
 (5) 29/01/2024
 Biologist Juan Ignacio Pérez Iglesias, UPV/EHU, DIPC

 Historian Joxean Fernández, Basque Film Archive
 Biologist Juan Ignacio Pérez Iglesias, UPV/EHU, DIPC

Subtitles and presentation in \*Spanish, \*\*French, and \*\*\*Basque.





The Perfect Storm (Wolfgang Petersen, 2000)\*\*\* (1) 01/02/2024 (2) 02/02/2024 (3) 23/03/2024 (4) 06/02/2024 Physicist Onintze Salazar, Euskalmet, Tecnalia Physicist Maialen Martija, Euskalmet, Tecnalia

Bombshell. The Hedy Lamarr Story (Alexandra Dean, 2017)\* (1) 08/02/2024 (2) 09/02/2024 (3) 10/02/2024 (4) 13/02/2024 Physicist Maia García-Vergniory, DIPC, Max Planck Institute for Chemical Physics of Solids Engineer Ane Insausti, Gipuzkoako Diputazioa, Mubil Fundazioa Engineer Mari Luz Guenaga, Universidad de Deusto Organized in collaboration with Emakumeak Zientzian

*Tiempo de Silencio* (Vicente Aranda, 1986)<sup>\*</sup> (1) 15/02/2024 (2) 16/02/2024 (3) 17/02/2024 (4) 20/02/2024 Biochemist Itziar Alkorta, UPV/EHU Chemist Fernando Cossío, UPV/EHU, Ikerbasque 

 Plan 75 (Chie Hayakawa, 2022)\*

 (1) 22/02/2024
 (2) 23/02/2024

 (3) 24/02/2024
 (4) 27/02/2024

 Physician Itziar Vergara, IIS Biogipuzkoa

 Organized in collaboration with Biogipuzkoa

 Bringing Up Baby (Howard Hawks, 1938)\*\*/\*\*\*

 (1) 29/02/2024
 (2) 01/03/2024

 (3) 02/03/2024
 (4) 05/03/2024
 (5) 04/03/2024

 Physicist Javier Aizpurua, DIPC, Ikerbasque
 Chemist Idoia Mujika, CFM (CSIC-UPV/EHU)

 Physicist Ricardo Díez Muiño, DIPC, Ikerbasque

Mars Express (Jérémie Périn, 2023)\*\*/\*\*\* (1) 07/03/2024 (2) 08/03/2024 (3) 09/03/2024 (4) 12/03/2024 (5) 12/02/2024 Engineer Amaia Bernaras, Euskadiko Parke Teknologikoa Physicist Ricardo Díez Muiño, DIPC, Ikerbasque

Theater of Thought (Werner Herzog, 2023)\* (1) 14/03/2024 (2) 15/03/2024 (3) 16/03/2024 (4) 19/03/2024 Physicist Aitzol García Etxarri DIPC, Ikerbasque



Representatives from different institutions at the presentation of the seventh edition of Cinema and Science.

### School Sessions

Special morning sessions were organized for high school students in San Sebastián and Bilbao. The selected film, "Mars Express" (Jérémie Périn, 2023) which calls for reflection on artificial intelligence, was presented by scientists from HiTZ Zentroa a reference center for language technologies that promotes research, training, technology transfer and innovation in artificial intelligence with a focus on language and speech.

### Tabakalera

Donostia/San Sebastián 28/02/2024\*\*\*

Presentations Computer Engineer **Rodrigo Agerri** HiTZ Zentroa - UPV/EHU

Computer Engineer Izaskun Etxeberria HiTZ Zentroa - UPV/EHU Bizkaia Aretoa UPV/EHU Bilbao 05/03/2024\*\*\*

Presentations Telecommunication Engineer Inma Hemáez HiTZ Zentroa - UPV/EHU

Telecommunication Engineer Jon Sanchez HiTZ Zentroa - UPV/EHU

### **ON ZIENTZIA**

DIPC and Elhuyar organized the 14th edition of the On Zientzia video contest. The aim of this competition is to promote the production and dissemination of short, original videos on science and technology for all types of audiences. This year we reached a new record of participation with 100 videos, submitted in Basque, Spanish, and English, with a good gender balance among the participants. Most of the entries came from the Basque Country but there were also videos from countries such as Argentina, Chile and Mexico.

The 2024 award ceremony was held on June 7 at Kutxa Fundazioa Plaza in Tabakalera.



In each category, the following videos were awarded:

### BEST DISSEMINATION VIDEO $\mathscr{O}$ El viaje de SiO<sub>2</sub>

Paula Alonso and Pablo Fernández

### BEST VIDEO IN BASQUE

 $\mathscr{S}$ Txantxangorri kuantikoa eta bestelako izaki maqikoak Jon Puignau

### YOUNG PRIZE

🔗 Dolly ardia Miren Ayerdi, Arhane Torres and Malen Irurzun

### SPECIAL MENTIONS

 $\mathscr{S}$  Adimen Artifiziala: funtzionamendua eta erronkak Maddi Piris *𝔗* Korronte ozeanikoez Patxi Juaristi

### AUDIENCE AWARD

 $\mathscr{O}$  Minaren sekretuak, ezagutzen dituzu? Noa Manso and Lydia Duro

To watch the videos visit

### WOMEN AND SCIENCE

The Women and Science program, launched by the Gipuzkoa Provincial Council and DIPC in 2021, aims to promote the presence of women of excellence in science, in line with DIPC's mission and the Council's objective to promote gender equality in all areas and especially in those where this inequality is most evident.

As part of this initiative, DIPC and the Gipuzkoa Provincial Council organized a seminar where Talat S. Rahman presented some programs that have helped the Physics Department at the University of Central Florida (UCF) to enhance diversity, equity and inclusion in its composition and mission.

Talat Rahman is a UCF Trustee Chair Professor and a Pegasus Professor of Physics. At UCF, she has been involved in efforts to increase the participation of women and minorities, particularly through the American Physical Society's Bridge Program, one of whose sites she helped establish at UCF with the goal of increasing the number of physics PhDs from underrepresented minority (URM) groups.

### IKUR QUANTUM TALKS

Leaders and specialists in guantum technologies from DIPC, UPV/EHU and BCAM organized the IKUR Quantum Talks series to raise awareness of the scientific foundation and potential of quantum technologies.

In 2024, two public lectures given by internationally renowned experts in the field were programmed, gathering around 200 attendees:

20/01/2024 San Telmo Museum Donostia/San Sebastián From atoms to stars: the universe according to Pauli Jean Philip Solovej Mathematician and mathematical physicist, University of Copenhagen Interview by Arantzazu García Lekue, DIPC, Ikerbasgue

08/03/2024 Bidebarrieta Auditorium, Bilbao Bell inequalities: from curiosity to security Artur Ekert Physicist, University of Oxford Interview by Luz Roncal, BCAM, Ikerbasque



22/03/2024 Diversity Matters – some strategies that could broaden participation Talat S. Rahman, University of Central Florida



### **JOT DOWN SCIENCE 2024**

03-04/05/2024 Tabakalera, Donostia/San Sebastián

For its 11th edition, after visiting Jaca and Sevilla, the Jot Down Science event returned to San Sebastián. This time it was organized by the cultural magazine Jot Down and DIPC, with the collaboration of Kutxa Fundazioa.

The 2024 edition focused on hominids-the primate family that includes modern humans (Homo sapiens), their direct ancestors, and other extinct relatives. The program featured a diverse range of formats, including lectures, interviews, and panel discussions with leading experts in paleoanthropology, archaeology, human evolution, physics, and geology.

As always, the event was also the scenario for the awards ceremony of the annual Jot Down Science popularization competition, in which DIPC has been collaborating since 2015. The contest currently includes four categories: scientific photography, scientific illustration, scientific dissemination essay and science fiction narrative. It is sponsored by Donostia International Physics Center (DIPC), the Laboratorio Subterráneo de Canfranc (LSC), the museum Laboratorium of Bergara and Jot Down with support from the Universidad de Sevilla, Mercurio Magazine, and Nextdoor Publisher.

### 03/05/2024

Lectures

Humanos, homínidos, y otros simios perdidos Emiliano Bruner, CENIEH, CIEN ¿Por qué surgió la agricultura? Amaia Arranz, UPV/EHU, Ikerbasque La espeleología. Última frontera de la exploración humana en la Tierra Sergio García Dils, International Cave Exploration Team CAVEX







### Round table on Art and Science

Clara Montero, Tabakalera, Mauricio Antón palaeoillustrator and Marina Otero, Columbia University GSAPP Moderator: Ángel L. Fernández, Jot Down

### 04/05/2024

Lectures Seducción cristalina Juan Manuel García Ruiz. DIPC, Ikerbasque, CSIC Por quién doblan las campanas. Violencia y evolución humana María Martinón-Torres, CENIEH

### Book presentation

Primates al este del edén by Juan Ignacio Pérez Iglesias, UPV/EHU, DIPC Interviewer: María Martinón-Torres, CENIEH



### Jot Down 2024 Science Outreach Contest

Best Scientific Dissemination Essay & Orce: piedras que se asemejan a huesos | Juan Manuel Jiménez Arenas

Best Science Fiction Narrative Award (joint winners) & Madres | Juan Carlos Pereletegui & Un edén improbable | Rebeca García Nieto

Best Scientific Illustration & El primer paso | Andrés Diam

Best Scientific Photography & Metamorfosis homínida | Jose Conceptes

### Lecture Una mirada a la evolución Conchi Lillo, Universidad de Salamanca Instituto de Neurociencias de Castilla y León, INCYL Book presentation

Nación Neanderthal by Juan José Gómez Cadenas, DIPC, Ikerbasque Interviewer: Ángel L. Fernández, Jot Down

The program also included complementary activities designed for children and families.

Workshop for children Animalien eboluzioa: lehoiak, oreinak, gorilak eta gizakiak Dynamisers: Jexux Tapia and Manu Ceberio, Aranzadi Zientzia Elkartea





12/04/2024 Barakaldo Theatre, Barakaldo La Cristalización de la Danza Dance lecture on art and science

### CRYSTALLIZATION OF DANCE

La Cristalización de la Danza (Crystallization of Dance) is an original proposal created by the crystallographer Juan Manuel García-Ruiz, and the dancer and choreographer Vanesa Aibar. The show invites us to reflect on their complementary visions of art, confronting the idea of abstraction, represented here by the inorganic and crystalline, with the empathy embodied by the biological and natural. The first performance in the Basque Country was in 2024:

### Vanesa Aibar, Dancer

Juan Manuel García-Ruiz, DIPC, Ikerbasque María Marín, Musician

### QUANTUM TECHNOLOGIES SERIES

Donostia is preparing to receive the world's sixth quantum supercomputer deployed by IBM, but what do we really know about this technology that could revolutionize science, education and industry?

The answer to these and other questions was tackled by the "Quantum Technologies" series, organized by DIPC and San Telmo Museoa in a new edition of *Donostia, Zientzia Hiria* initiative which was attended by over 150 people. This annual collaboration is part of the 'Challenges' program at San Telmo Museoa.



In 2024, the series included the following:

19/04/2024 *Teknologia kuantikoak: zer da hori?* **Javier Aizpurua**, BasQ, DIPC, Ikerbasque

### 26/04/2024 Acercándonos a las tecnologías cuánticas Celia Rogero, CFM (CSIC-UPV/EHU) Kepa Ruiz Mirazo, UPV/EHU and Biophysics Institute Aitor Moreno, Ayesa Cristina Sanz, IBM Moderator: Javier Aizpurua, BasQ,

DIPC, Ikerbasque



### SCIENCE WEEK

07-09/11/2024 Tabakalera

Once again, DIPC participated in the Science Week of the University of the Basque Country (UPV/EHU), together with CIC nanoGUNE, the Materials Physics Center (CFM CSIC-UPV/EHU) and POLYMAT research centers.

In 2024, researchers from the four centers led the usual stand with hands-on experiments in materials science and nanoscience, which was open to the public in the "Txokos" section. In addition, the program included two workshops; the already classic one for children focused on experimenting and visualizing the tiny world, and a new workshop developed in collaboration with the experimental particle physics researchers from DIPC.

07-09/11/2024 Stand "Exploring the world of materials"

08/11/2024 Zientzia Club Diamonds are (quantum) physics' best friends Gabriel Molina CFM, Ikerbasque, DIPC

08/11/2024 Cosmic Rays and Elementary Particles Workshop for schools (12-16 years old)

09/11/2024 Scale your World Workshop for children (4-8 years old)

### Screening of EL SECRETO DE LA NATURALEZA

El secreto de la naturaleza (José Antonio Pérez Ledo, 2018) is a documentary film co-produced by the Chair of Scientific Culture of UPV/EHU and K2000 which traces the life and scientific legacy of Pedro Miguel Echenique through his reflections on science and beauty. Two screenings were organized in 2024:

### 12/09/2024

Tabakalera, Donostia/San Sebastián

The Basque Film Archive and the Chair of Scientific Culture of the UPV/EHU organized the screening in San Sebastian. Juan Ignacio Pérez Iglesias, Minister of Science, Universities and Innovation, and Joxean Fernández, Director of the Basque Film Archive, introduced the film. After the screening, Prof. Echenique was interviewed by Edurne Ormazabal, general director of Tabakalera, and answered the questions from the audience. The screening was organized in collaboration with DIPC and the San Sebastian International Film Festival.

### 15/11/2024

San Agustin Kulturgunea, Durango

The documentary was screened as part of the "Zientziaren Ertzetik" series of scientific talks, and was supported by Durango City Council, Bizenta Mogel Library, the Chair of Scientific Culture of the UPV/EHU, DIPC and the Basque Government. After the screening Pedro Miguel Echenique and Jone Guenetxea, director of the weekly magazine Anboto, led a colloquium.



### SESSIONS FOR KIDS: San Sebastián International Film Festival

20, 23-27/09/2024 Ikastetxeak Belodromoan, Anoeta Velodrome



As part of the San Sebastian International Film Festival (SSIFF), thousands of children between the ages of 6 and 11 come together to enjoy children's film screenings. Co-organized by SSIFF, DIPC, and the Basque Film Archive since 2019, the initiative aims to promote a positive image of science among local schoolchildren, highlighting the city's strong ties to scientific research. The slogan City of Cinema, City of Science reflects this goal.

This time round, Ikastetxeak Belodromoan focused on extraterrestrial life. The Velodrome's giant screen showed Little Allan – The Human Antenna (Alan giza antena), a Danish animated movie directed by Amalie Næsby about the relationship between a little alien girl and an 11-year-old boy and his UFO-obsessed neighbor. The screening of the film, dubbed into Basque, included an original introduction with several surprises.

This year's invited scientist was astrophysicist Naiara Barrado from the Planetary Sciences Group of the Bilbao School of Engineering (UPV/EHU). Together with Naiara, the Velodrome embarked on a journey through the universe trying to answer the big guestion about the existence of extraterrestrial life.



One of the surprises was the return of the already 'famous' social robot Pepper and his new friend Aatxe, a guadruped robot with all kinds of acrobatic skills. This special session was made possible thanks to the collaboration of Elena Lazkano, Igor Rodriguez, Unai Zabala and Eneko Atxa, members of the robotics research group Robotics and Autonomous Systems (RSAIT) from the University of the Basque Country (UPV/EHU). At the end of the event, there was a real party where Pepper and Aatxe danced together with an enthusiastic audience.

### Premier of OLATU BATEN ISTORIOA

### 12/11/2024 Bilbao

The Bilbao Zinebi International Documentary and Short Film Festival presented the premiere of Olatu Baten Istorioa (The Story of a Wave), a short film produced by El Santo Films and directed by Nagore Eceiza which explores the connection between the physics of waves and the passion for surfing.



### EL PALO DE ERATÓSTENES – ZIENTZIA ELKARRIZKETAK

Aranzadi Science Society continued the lecture series El Palo de Eratóstenes – Zientzia Elkarrizketak during 2024 in collaboration with Eureka! Zientzia Museoa and DIPC.

The series was named after the scientist Eratosthenes who, 2,000 years ago, measured the circumference of the Earth using the shadow cast by a stick. It is a science outreach program focusing on astronomy, astrophysics, cosmology and other scientific fields.

The following scientists participated in the series organized from March to June:

14/03/2024 Ignacio Tanco, ESA 09/04/2024 Silvia Bonoli, DIPC, Ikerbasque 14/05/2024 Eduardo Zubia, Aranzadi 11/06/2024 Raúl Angulo, DIPC, Ikerbasque

The film features the surfer Kepa Acero and includes the scientific collaboration of the physicist Maia García-Vergniory, researcher at DIPC and at the time, professor of condensed matter physics at Sherbrooke University in Canada.

This interdisciplinary project has its origins in Donostia, Zientzia Hiria initiative, promoted by DIPC, the Chair of Scientific Culture of the UPV/EHU and Donostia Kultura. Its first edition in 2022, focused on Surf and Science and included the participation of Kepa Acero and Maia García Vergniory with a joint lecture entitled Olatu Baten Istorioa (The Story of a Wave). Two years later the short film of the same name was born.

The production was possible thanks to the support of the Basque Government, Fundación EDP, DIPC, Euskampus and the Chair of Scientific Culture of the UPV/EHU.



### HIGH SCHOOL VISITS

For the tenth consecutive year, DIPC and the Materials Physics Center (CSIC-UPV/EHU) organized the well-established DIPC/CFM Visits Program. The aim of the program is to promote scientific careers among young students by showing them our daily activity, the research areas we work in and our facilities. To carry out this activity, we count on scientists who volunteer to show their work and accompany the visitors during the 2-hour visit. In 2024, six on-site visits and two virtual visits were scheduled, one of them held as part of the Emakumeak Zientzian initiative. A total of 25 high schools and 1,160 students were hosted during the year.

In addition, two special visits were organized as part of UPV/EHU's orientation program Eqokitu, and students from the Computer Science Faculty of UPV/EHU and Universidad Europea paid a special visit to the DIPC Supercomputing Center. Moreover, winners of Elhuyar Zientzia Azoka visited our research center.

### STRØM - Inclusive Astronomy

The STRØM – Inclusive Astronomy exhibition, created by DIPC for Passion for Knowledge 2023, was inaugurated at the Pamplona Planetarium in December 2024 as part of a collaboration agreement signed between the two institutions.

The Pamplona Planetarium is the first institution after Tabakalera in San Sebastian, to host this touring exhibition which invites visitors to explore the cosmos through tactile, sound and audiovisual experiences with the aim of guaranteeing access to science for all citizens without barriers of any kind.



From left to right: Paula Noya (NICDO), Patricia Fanlo (Government of Navarre), Pedro Miguel Echenique (DIPC, UPV/EHU), Izaskun Azcona (Fundación La Caixa) and Silvia Bonoli (Ikerbasque, DIPC). The opening ceremony was attended by Paula Noya, Head of Cultural Infrastructures of NICDO; Patricia Fanlo, regional minister for Universities, Innovation and Digital Transformation of the Government of Navarre; Izaskun Azcona, La Caixa Foundation's representative in Navarre; Pedro Miguel Echenique, president of DIPC and professor emeritus of the University of the Basque Country (UPV/EHU), and Silvia Bonoli, Ikerbasque research professor at DIPC and scientific curator of STRØM.

From the inauguration, on December 19, to the last day of 2024, the exhibition received a total of 970 visitors, of which 84 were guided tours and 886 were members of the general public.

As a result of a fire that affected the Pamplona Planetarium's dome, the exhibition will be relocated in 2025, with the hope of reopening to the public in Pamplona.

### top@DIPC ENCOUNTERS Zientziarekin Solasean

On November 28, we celebrated the XIV edition of top@DIPC Zientziarekin Solasean! at Eureka! Zientzia Museoa, an event that brings together top-level scientists and high school students from the Basque Country.

In this edition, the students had the opportunity to interact with Nobel Laureate Jean-Pierre Sauvage, the president of the European Physical Society, Mairi Sakellariadou, and the vice-president of the CERN Science Policy Committee, Pilar Hernández. The physicist and DIPC's president Pedro Miguel Echenique moderated the discussion, during which the invited scientists shared insights into their professional careers and answered the students' questions.

The main objective of this gathering is to encourage young people in the Basque Country to pursue studies in science and technology, and to instill a passion for knowledge. DIPC organized the event, with the support of the Department of Science, Universities and Innovation of the Basque Government and Kutxa Fundazioa, as well as the special collaboration of Telefónica, which awarded the prize for the most in teresting and original question among the participants



Eureka! Zientzia Museoa in Donostia/San Sebastián.

28/11/2024 Eureka! Zientzia Museoa Jean-Pierre Sauvage, Université de Strasbourg Mairi Sakellariadou, King's College London Pilar Hernández, Universitat de València, IFIC, CERN Moderated by Pedro Miguel Echenique, President of DIPC



Students and teachers from around the Basque Country gather at the XIV edition of top@DIPC Encounters in front of the

Hosts:

Ander Aizpurua, General Director of Kutxa Fundazioa Javier Benito, Director of Telefónica Euskadi Adolfo Morais, Vice-minister of Universities and Research, Department of Science, Universities and Innovation of the Basque Government

### NEW PATHS OF SCIENCE

Co-organized by the Ernest Lluch Cultural Center of Donostia Kultura and DIPC, the aim of this series of lectures is to bring the research done by local scientists closer to citizens. This year, two talks were held and gathered over 75 attendees.

The lectures are available in podcast format at Donostia Kultura Irratia.

### 22/10/2024

Arantzazu García Lekue, DIPC, Ikerbasque



### 26/11/2024

 $\mathscr{O}$  Mapeando la cultura. Enredando ciencias y humanidades Gustavo Ariel Schwartz, CFM CSIC-UPV/EHU. DIPC

### MESTIZAJES

During 2024, the Mestizajes project has continued to foster dialogue between science, literature, and the other branches of 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 research and outreach activities such as conferences, seminars, presentations or collaborative projects have been carried out during the last 14 years. These activities have been organized in collaboration with Donostia Kultura, Tabakalera and the Vice Rectorate of the Gipuzkoa Campus of the University of the Basque Country (UPV/EHU).

In 2024, research on complex networks applied to cultural analytics has continued actively through our collaboration with The CulturePlex Lab (Canada), which began in 2021. This interdisciplinary project explores the emergence of genius and revolutionary ideas using data mining, complex network analysis, and machine learning. By modeling cultural networks around iconic figures and transformative moments -such as the early 20th-century intersections of art, science, and literature- the project bridges quantitative analysis with traditional humanities research.

### OTHER COLLABORATIONS

In addition to our outreach program, we sponsor and support various initiatives every year thanks to the participation of our researchers. In 2024, these initiatives include: Inspira Bizitzak, organized by Kutxa Fundazioa to inspire new generations of students to pursue scientific careers; Pint of Science, an international initiative featuring informal talks by local scientists in bars around the city; the Scientific Bidebarrieta cycle, organized by the Chair of Scientific Culture of UPV/EHU and the Bidebarrieta Library; the special event Machine Learning application in streaming platforms organized by DIPC and Kutxa Fundazioa; and the presentation of the documentary El misterio de los cristales gigantes at the 36th Urrelur Mineralogy and Paleontology Week.

### **STEAM SARE: Gravitating Bodies**

In the framework of the STEAM Euskadi strategy, promoted by the Department of Education of the Basque Government through Innobasque, DIPC participated in 2022, in the co-creation of the activity "Gravitating Bodies", in collaboration with teachers from the Ikastola Lauaxeta (Bizkaia) and the artist Saioa Olmo.

The pilot test of this activity was carried out by DIPC post-doctoral researchers Marcos Pellejero and Sergio Contreras, and took place at the Lauaxeta center. After a positive assessment by the teaching staff, "Gravitating Bodies" became part of the STEAM Sare catalog of activities offered to secondary and high school students in the Basque Country. In 2024, the activity was led by DIPC researchers Sergio Contreras, Irati Lizaso, Sara Ortega and Irene Valderrama, in the following schools:

29/02/2024 Ategorri BHI, Erandio, Bizkaia 15/11/2024 Lauaxeta Ikastola, Amorebieta-Etxano, Bizkaia 26/11/2024 Nazaret, Donostia/San Sebastián, Gipuzkoa

### **DONOSTIA WeekINN 2024**

### 25-31/10/2024

As every year, DIPC collaborated in the Innovation Week "Donostia WeekINN" organized by Fomento of San Sebastián.

As part of the 2024 edition, CFM and DIPC research centers offered a materials science workshop conducted by researchers from both institutions. DIPC also participated in a special event that brought together citizens and R+D+i agents to discuss the social impact of science: San Sebastian Science Society.







28/10/2024 Kursaal

Ciencia con Impacto Social, ¿cómo lo definimos? Javier Aizpurua, BasQ, Ikerbasque, DIPC

29/10/2024 Santo Tomas Lizeoa *Materials Science Workshop* for students by CFM and DIPC Irene Vittori, Marco Gobbi and Shayan Edalatmanesh

# Equality at DIPC

In 2024, we continued to advance gender equality through various projects and initiatives. The Emakumeak Zientzian alliance has strengthened networks, raised awareness, and made a meaningful impact on society through a diverse program of activities around February 11th, the International Day of Women and Girls in Science.





Presentation of Emakumeak Zientzian 2024.

### **Emakumeak Zientzian**

Emakumeak Zientzian is a strategic equality project in the Basque Country that has received several awards. It has been promoted by DIPC since its inception and has successfully expanded its network of partners. In 2024, 32 Basque institutions joined forces to organize the International Day of Women and Girls in Science, which is celebrated on February 11th. These institutions have committed themselves to the objectives of the initiative by signing a cooperation agreement. The aim is to showcase the activities of women in science, to break gender stereotypes in scientific and technical fields, and to encourage girls and young women to pursue scientific careers. The program has successfully achieved its goals through the implementation of 65 aligned actions, involving **13,500 people** of all ages, including children, teenagers, and adults. It is estimated that in its 8 editions, the Emakumeak Zientzian project has had a significant social impact, reaching more than **30,000 people** in the Basque Country.

### **DIPC Equality Plan**

The first DIPC Equality Plan was launched by DIPC in 2020. It was designed as a framework consisting of four main areas identified as key challenges during the diagnostic process: organizational culture, workforce diversity, sexual harassment in the workplace, and work-life balance. One of our main goals at DIPC is to foster an inclusive organizational culture with gender-diverse leadership and transparency at its core. Each year, we share significant actions with the community to reinforce our commitment.

In addition, we recognize the importance of promoting diversity and inclusion internally by implementing inclusive language across various communication channels. To promote a diverse workforce, we have raised awareness and increased the visibility of underrepresented researcher collectives (gender, ethnic background, etc.) as role models in local community events.

Furthermore, in 2024, we continued the special "Women and Science" program, created in partnership with the Gipuzkoa Provincial Council, to promote the careers of outstanding female scientists. In 2021, a protocol was established to ensure and maintain a dignified working environment for all DIPC employees, free from violence of any kind, including violence against women and minorities. This applies both within and outside the physical space of DIPC, as well as to instances occurring through virtual or symbolic means of communication. The implementation of this Protocol, which has been in place for three years, represents one of the most significant milestones of our Gender Equality Plan. Every year, awareness and prevention campaigns are carried out with the active participation of our community.



Looking ahead to next year, one of our key challenges will be the renewal of our First DIPC Equality Plan and the subsequent development of the Second DIPC Equality Plan. This new plan, spanning the next four years, will strengthen our commitment to diversity, equity, and inclusion. We will achieve this by implementing impactful initiatives, raising awareness, and ensuring fair and inclusive practices across DIPC.

00		
	Total Staff	
Direction and Management		
Directors	1   <mark> </mark>	
Management	6   <mark>C</mark>	
Total	7   <mark>C</mark>	
Scientists		
Early Stage Researchers	77   <mark>C</mark>	
Post-doctoral Researchers	60   <b>C</b>	
Permanent Researchers	30   <mark>C</mark>	
Research Fellows	7   <mark>C</mark>	
Technical Support	10   <mark>0</mark>	
Total	184   <mark>C</mark>	
Administration and Services		
Administration	11   <b>C</b>	
IT Personnel	9   <b>C</b>	
Outreach Personnel	4   <mark>∎</mark>	
Maintenance	2   <mark>6</mark>	
Projects	4   <mark>C</mark>	
Total	30   <b>C</b>	
TOTAL	221 C	

### **Associates and Visiting Researchers**

	Total Staff		
DIPC Associates		72	
Visiting Researchers		210	C  C

Data as of 31/12/2024. DIPC includes the non-binary gender definition, but none has been recorded to date.



Enantiopure [6]-azairidahelicene by dynamic kinetic of a configurationally labile [4]-helicene...

Thermoelectric properties of the main species pres

Mixed stereochemistry macrocycle acts as a helix-

Interfacing two-dimensional and magnetic topolog Bi bilayer on MnBi<sub>2</sub>Te<sub>4</sub>-family materials...

Enhancing haloarene coupling reaction efficiency

Impact of single-melamine tautomerization on the molecular vibrations in inelastic electron tunneling

Deceptive orbital confinement at edges and pores

Uncovering low-frequency vibrations in surface-en

On-chip phonon-enhanced IR near-field detection

Fluorescence imaging of individual ions and molec pressurized noble gases for barium tagging in <sup>136</sup>Xe

A deep learning method that identifies cellular hete

Efficient near-infrared organic light-emitting diodes

Bending rigidity, sound propagation and ripples in

Detection of a universal core-halo transition in dwa as predicted by Bose-Einstein dark matter ....

Indistinguishability of identical bosons from a quan

Universal features of entanglement entropy in the

Evolution of superconductivity in twisted graphene

Catalog of topological phonon materials...

Morphological sensitivity to pH of silica and chalk

# Scientific Highlights

ic resolution	
	34
sent in Portland cement pastes	36
stabilizing peptide N-cap	38
gical insulators:	40
on an oxide surface by metal atom addition	42
e excitation of g spectroscopy	44
of carbon-based 1D and 2D nanoarchitectures	46
nhanced Raman Scattering of organic molecules	48
n of molecular vibrations	50
cules in /e	52
erogeneity using nanoscale nuclear features	54
s with emission from spin doublet excitons	56
flat graphene	58
arf galaxies	
	60
ntum information theory perspective	62
honeycomb Hubbard model	64
e multilayers	66
	68
nanocrystalline self-organized biomorphs	70

# Enantiopure [6]-azairidahelicene by dynamic kinetic resolution of a configurationally labile [4]-helicene

Pazos A, Cruz CM, Cuerva JM, Rivilla I, Cossio FP, and Freixa Z *Angewandte Chemie International Edition 63*, e202406663 (2024)

"Helicene" is the name introduced by Newman in 1955, to describe the benzologues of phenanthrene in which the extra ortho-condensed rings give rise to a (regular) cylindrical helix. The pioneer work of Newman in this field cannot be overemphasized; his brillant synthesis and resolution of [6]helicene will remain as a landmark, for it opened the way to the study of a fascinating class of synthetic molecules.

**Formally, helicenes are ortho-fused** polycyclic aromatic or heteroaromatic compounds in which all rings (minimum five) are angularly arranged so as to give helically shaped molecules, which are thus chiral. This chirality results from the handedness of the helicity itself, lacking both asymmetric carbons and chiral centers. The clockwise and counterclockwise helices are non-superposable. By convention, a left-handed helix is minus and labelled (M), a right-handed helix is plus and labelled (P). The chemistry of helicenes has attracted continuing attention because of their unique structural, spectral, and optical features.

Organometallic helicenes are appealing chiral entities. By combining the chiroptical properties of helicenes with those inherent to the metal centre, they are suitable for the development of multifunctional molecules. Among them, few examples of iridahelicenes appeared in the literature, intended to exploit the outstanding photophysics of iridium(III) bis- or tris cyclometalated complexes, combined with the central chirality imposed by the organometallic core and the helicenic structure.

Now, a team of researchers reports the synthesis of a pair of enantiopure [6]-azairidahelicenes incorporating chirality at the metal center and on the helicenic ligand. These two organometallic helicenes are readily accessible by an effective dynamic kinetic resolution (dkr) of a configurationally labile [4]-helicenic ligand. The two isolated enantiomers exhibit perfect mirrored electronic circular dichroism (ECD) and circularly polarized phosphorescence (CPP) signals.

According to the results, dkr is strongly directed by structural features on the reaction intermediates towards cyclometalation, imposed by the  $C_2$ -symmetric bis-cyclometalated organometallic core. This type of arrangement is common in many organometallic compounds. Consequently, this synthetic strategy can be extended to obtain not only a variety of chiral [6]-azairidahelicenes but also other metallahelicenes by simple combinations of ready-available chiral-at-metal bis-chelated precursors conformationally stable and epimerizable [4]-helicene derivatives.



Cover image of the issue, representing the enantiomeric irida[6]helicenes exhibiting perfect mirrored electronic circular dichroism (ECD) and circularly polarized phosphorescence (CPP) signals.



Enantiopure irida [6]helicenes combining chirality at the metal center and at the helicenic fragment are obtained by dynamic kinetic resolution of configurationally labile [4]helicenic ligands



# Thermoelectric properties of the main species present in Portland cement pastes

Agbaoye RO, Janovec J, Ayuela A, and Dolado JS Sement and Concrete Research 183, 107587 (2024)

In the pursuit of sustainable energy solutions, thermoelectricity offers a compelling pathway converting wasted heat into usable electrical energy. While promising, its success hinges on enhancing the efficiency of thermoelectric materials.

Cement and concrete, despite their ubiquity, remain under-explored in this context, with reported figures of merit still lingering between  $10^{-7}$  and  $10^{-9}$ . Unlocking their energy-harvesting potential requires improving the intrinsic thermoelectric properties of their core components. Notably, portlandite and tobermorite-11 exhibit inherently low lattice thermal conductivity, a critical advantage that significantly boosts their thermoelectric performance and positions them as promising candidates for next-generation smart construction materials.

Tobermorite-11, a key mineral found in cement, has shown unexpected promise as a thermoelectric material capable of converting heat into electricity. Within a hole carrier concentration range of  $10^{20}$  to  $10^{21}$  cm<sup>-3</sup>, it delivers an impressive Seebeck coefficient of up to  $400 \,\mu$ V/K, and a thermoelectric figure of merit (Z) between 0.5 and 0.79 across a practical temperature window of 350 K to 600 K. To enhance these properties, we explored p-type doping by replacing a silicon atom in the tobermorite structure with aluminum. This substitution introduces one hole per unit cell, effectively reaching an ideal carrier concentration of 10<sup>21</sup> cm<sup>-3</sup> and achieving a Z value of 0.5 at 600 K. However, while adding more aluminum increases electrical conductivity, it comes at a cost reducing both the Seebeck coefficient and

the overall efficiency. Our findings reveal that optimal performance is achieved when one silicon atom is replaced by aluminum in every ten unit cells, maintaining a balance between conductivity and thermoelectric efficiency. These insights highlight a powerful strategy: through selective n- and p-type doping, we can engineer cement-based materials not just to build, but to actively harvest energy transforming concrete into a functional component of sustainable, energy-aware infrastructure.



Hole carrier concentration-based thermoelectronic properties of normal tobermorite-11.



Crystal structures of Ca(OH)<sub>2</sub> and normal tobermorite-11.

With precise p-type doping-elegantly replacing silicon with aluminum in tobermorite, we unlock a dramatic rise in performance

The result: A bold leap toward energy-harvesting cement composites that redefine what infrastructure can do



# Mixed stereochemistry macrocycle acts as a helix-stabilizing peptide N-cap

Hink F, Aduriz-Arrizabalaga J, Lopez X, Suga H, De Sancho D, and Roger JM & Journal of the American Chemical Society 146, 24348 (2024)

Peptides are a promising class of compounds for inhibiting protein-protein interactions, as they can mimic the behavior of natural intrinsically disordered proteins (IDPs). However, short linear peptides typically lack a defined structure in isolation and must fold upon binding, which incurs an entropic penalty that reduces binding affinity.

Macrocyclization - the formation of rings containing twelve or more atoms- has emerged as an effective strategy to "preorganize" peptides by stabilizing their bioactive conformations, particularly a helices. In addition to rational design approaches, the RaPID system (Random non-standard Peptides Integrated Discovery) enables the discovery of de-novo macrocyclic peptides from genetically reprogrammed libraries incorporating non-canonical amino acids. While most peptides identified by the RaPID system adopt coil or sheet-like conformations, only a few form  $\alpha$ -helices. This raises the question of whether such short N-terminal-to-side-chain macrocycles can effectively mimic longer helical motifs.

To investigate this question, a research team composed of experimentalists from the University of Copenhagen and computational chemists from DIPC and UPV/EHU focused on Mcl-1 - a clinically relevant apoptosis regulator and member of the Bcl-2 protein family that recognizes a-helical BH3 motifs from pro-apoptotic proteins such as Bid. Using the RaPID system, they identified potent binders, termed "Heliats", which feature a four-residue macrocycle (formed via a thioether bond) fused to a short linear segment that mimics BH3 motifs. These Heliats bound Mcl-1 with nanomolar affinity and effectively disrupted its interaction with native ligands. Notably, macrocyclization was found to both enhance binding affinity and promote  $\alpha$ -helical structure.

Computational studies conducted by the DIPC and UPV/EHU team provided detailed mechanistic insights into the stabilization effect. Molecular dynamics simulations demonstrated that macrocyclization increased  $\alpha$ -helical content compared to linear analogs, particularly near the macrocyclic region, and promoted key i to i+4 hydrogen bonds. Quantum chemical calculations corroborated the presence of these interactions, especially involving the D-stereocenter at position 1, which adopted polyproline II torsion angles conducive to helix stabilization and thioether linkage formation. The simulations also revealed that this D-stereochemistry favors macrocyclic geometries and intramolecular hydrogen bonding, effectively pre-organizing the peptide for target binding. Together, these findings underscore the utility of a minimal, mixed-stereochemistry macrocyclic N-cap that is synthetically accessible and broadly graftable - offering a versatile platform for helix stabilization and improved peptide-protein interactions in drug discovery.



Torsional distribution of Ramachandran angles for the L-Phe and D-Phe variants.

Researchers have developed "heliats", peptides that mimic a-helical motifs to block protein-protein interactions, with simulations revealing how macrocyclization enhances both structural preorganization and binding affinity





# Interfacing two-dimensional and magnetic topological insulators: Bi bilayer on MnBi<sub>2</sub>Te<sub>4</sub>-family materials

Klimovskikh II, Eremeev SV, Estyunin DA, Filnov SO, Shimada K, Golyashov VA, Solovova NY, Tereshchenko OE, Kokh KA, Frolov AS, Sergeev AI, Stolyarov VS, Trontl VM, Petaccia L, Di Santo G, Tallarida M, Dai J, Blanco Canosa S, Valla T, Shikin AM and Chulkov EV *Materials Today Advances 23*, 100511 (2024)

Recently observed axion quasiparticle in Chern insulator  $MnBi_2Te_4$  ignites its use for dark matter detector. Heterostructuring of  $MnBi_2Te_4$  with another topological insulator, 2D bismuth layer, extends the applications even broader, possibly resulting in high and tunable Chern number systems.

**Discovery of non-trivial topological phases** opened one of the most fruitful area in solid state physics and chemistry. Recently, it was shown that when the non-trivial topology meets magnetism, new phases and phenomena, such as Quantum Anomalous Hall Effect (QAHE) and Majorana zero modes emerge. QAHE in the first 3D intrinsic magnetic topological insulator (IMTI), MnBi<sub>2</sub>Te<sub>4</sub>, with Chern number (C = 1) was greatly enhanced, but further gain is expected for magnetic topological heterostructures. Recently, intriguing possibility of tunable QAHE with high and tunable Chern numbers ( $C = \pm 1, \pm 3$ ) was predicted for heterostructures consisting of 2D topological insulators and IMTIs.

The Chern number corresponds to the number of the 1D gapless chiral modes residing at the Chern insulator film's edge. These edge modes conduct electricity without dissipation, which could be useful for the construction of novel highly efficient chiral interconnects for low-power-consumption electronics. However, the contact resistance between a metal electrode and Chern insulator in the envisioned interconnect devices is a bottleneck limiting their performance. To reduce this resistance as much as possible, the number of chiral edge modes should be as large as possible. Therefore, it is of great interest and importance to engineer TIs with high Chern numbers.

We have synthesized and characterized the heterostructures consisting of 2D topological insulator Bi bilayer (Bi-BL) and IMTIs in the  $MnBi_2Te_4$  family. Using angle-resolved photoemission spectroscopy (ARPES), the electronic structure of the interface is detected that uncovers the interaction of the substrate surface states with the Bi-BL states, in agreement with our DFT calculations. Further, our calculations predict exchange-split 1D topological states at the Bi-BL edges that may result in a number of intriguing quantum phenomena beyond the high temperature QAHE, such as TRS-broken QSHE phase and tunable Chern number system.



ARPES dispersion relations in the low energy region in the K –  $\Gamma$  – K direction of BZ of MnBi<sub>2</sub>Te<sub>4</sub>-family samples taken at 17 K before (upper panels) and after (lower panels) Bi deposition. The photon energies are 20 eV for (a,d,e,f,h), 9 eV for (b), 30 eV for (c,g).



Side view of the atomic structure of Bi-BL ribbon on top of MnBi<sub>2</sub>Te<sub>4</sub> and spacial charge distribution of the 1D states calculated by means of DFT. ARPES measurements of the MnBi<sub>2</sub>Te<sub>4</sub> surface before and after Bi-BL deposition are shown at the inset with super-imposed DFT bandstructure.



Magnetic topological substrate "transfers" its unique properties to 2D bismuth film on top

# Enhancing haloarene coupling reaction efficiency on an oxide surface by metal atom addition

Abadia M, Piquero-Zulaica I, Brede J, Verdini A, Floreano L, Barth JV, Lobo-Checa J, Corso M, and Rogero C *Nano Letters 24*, 1923 (2024)

This study presents a new strategy for implementing the on-surface Ullmann-like reaction with high efficiency on poorly reactive semiconducting or insulating surfaces such as  $TiO_2(110)$ , opening a promising avenue for synthesizing graphene-based nanostructures, such as graphene nanoribbons and nanoporous graphene structures, directly on more technologically relevant surfaces.

**Throughout the past decade,** on-surface chemistry has proven to be an extraordinary tool for building sp<sup>2</sup> bond-based carbon nanostructures with unprecedented atomic precision. Motivated by the fact that such carbon structures, which are hard to synthesize by common wet chemistry methods, have prominent electronic properties deserving implementation into electronic devices, the interest of exploring surface-induced molecular reactions has grown exponentially.

The Ullmann coupling reaction, in conjunction with a subsequent cyclodehydrogenation step, is recognized as the most promising pathway toward designing carbon-based nanostructures for molecular electronics on surfaces. However, bringing such materials into nanodevices remains a challenge, as the surface-assisted Ullmann reaction is mostly employed in ultrahigh vacuum (UHV) conditions on single-crystal noble metal substrates (gold, silver, and copper) given their catalytic activity. Nevertheless, these metal-adsorbed nanostructures present limitations since they remain electronically coupled to the underlying catalyzing substrate. Thus, the decoupling of the synthesized nanostructures must be achieved afterward for their implementation into devices, which is currently performed by cumbersome post-growth transfer methods.

The bottom-up synthesis of carbon-based nanomaterials directly on semiconductor surfaces allows for the decoupling of their electronic and magnetic properties from the substrates. However, the typically reduced reactivity of such nonmetallic surfaces adversely affects the course of these reactions.

Now, a team of researchers achieve a high polymerization yield (it is practically tripled) of halogenated polyphenyl molecular building blocks on the semiconducting  $TiO_2(110)$  surface via concomitant surface decoration with cobalt atoms, which catalyze the Ullmann coupling reaction.



On the top, the components involved in the on-surface Ullmann coupling reaction are shown: DBTP as the molecular precursor, cobalt as the external catalyst, and  $TiO_2(110)$  as the template substrate. On the bottom, the adsorption of DBTP on the  $TiO_2(110)$ .

# Metal additions boost key surface chemical reactions for future technologies

Specifically, cobalt atoms trigger the debromination of 4,4"-dibromo-p-terphenyl molecules on  $TiO_2(110)$ and mediate the formation of an intermediate organometallic phase already at room temperature. As the debromination temperature is drastically reduced (lowered by 55 K), homocoupling and polymerization readily proceed, preventing presursor desorption from the substrate and entailing a drastic increase of the poly-para-phenylene polymerization yield. The general efficacy of this mechanism is shown with an iodinated terphenyl derivative, which exhibits similar dehalogenation and reaction yield.



# Impact of single-melamine tautomerization on the excitation of molecular vibrations in inelastic electron tunneling spectroscopy

Alkorta M, Cizek R, Neel N, Frederiksen T, and Kroeger J 

Understanding how molecular transformations affect quantum properties at the atomic scale is essential for advancing nanoscale electronics and surface chemistry. This study investigates how tautomerization in single melamine molecules modulates vibrational spectra using STM-IETS.

The reversible switching of a single melamine molecule on a copper surface reveals how minute changes in chemical structure can lead to measurable shifts in quantum mechanical behavior. Using inelastic electron tunneling spectroscopy (IETS) in a scanning tunneling microscope (STM), researchers observed significant changes in low-energy vibrational spectra following a tautomerization reaction- a subtle proton transfer within the molecule. This reaction, triggered by electron injection or by bringing the probe tip into contact with the molecule, alters the symmetry of the molecule and thereby modulates its inelastic electron scattering signature.

Key to the discovery is the identification of a redshift in an internal bending vibrational mode upon tautomerization, supported by detailed simulations. These changes are not merely structural curiositiesthey demonstrate how electronic transport and vibrational coupling in a molecular junction are governed by both molecular conformation and the local electronic environment. Notably, forming a chemical bond between the scanning tip and the molecule not only guenched the inelastic signal but also effectively drove the tautomerization, suggesting a method to control molecular states mechanically and electronically.

Combining experimental scanning tunneling spectroscopy with advanced transport calculations allowed the researchers to pinpoint the active vibrational modes and identify symmetry rules that govern the observed signal changes. These findings provide foundational insights for designing molecular devices with switchable properties and contribute to our understanding of fundamental processes in singlemolecule electronics.

Beyond its implications for molecular electronics, this study underscores the strength of combining precise experimental manipulation with theory driven interpretation in surface science. The ability to reversibly switch molecular states and resolve their vibrational signatures with sub-millivolt resolution showcases how far scanning probe techniques have advanced. The observed sensitivity of vibrational spectra to subtle structural and bonding changes highlights the value of IETS as a powerful diagnostic for probing reaction pathways at the atomic level. That bond formation with the STM tip can initiate tautomerization further demonstrates how mechanical and electronic interactions can be harnessed to explore chemical reactivity with single-molecule precision. Together, these results reflect significant strides in understanding and manipulating molecular behavior on surfaces.



Cover image from Nano Letters illustrating a transport scattering state across a melamine molecule on Cu(100) contacted with an atomically sharp STM tip.

Mechanically induced switching: Bonding the STM tip to the molecule triggers a reversible chemical transformation, paving the way for controllable molecular junctions



# Deceptive orbital confinement at edges and pores of carbon-based 1D and 2D nanoarchitectures

Piquero-Zulaica I, Corral-Rascón E, Diaz de Cerio X, Riss A, Yang B, Garcia-Lekue A, Kher-Elden MA, Abd El-Fattah ZM, Nobusue S, Kojima T, Seufert K, Sakaguchi H, Auwärter W, and Barth JV *Nature Communications 15*, 1062 (2024)

Over the past decade, on-surface chemistry has enabled the atomically precise synthesis of target carbon-based nanoarchitectures, such as graphene nanoribbons and nanoporous graphene structures. The electronic properties of these materials are highly sensitive to single-atom variations in their atomic structure and chemical composition, making atomic-scale characterization tools essential.

Scanning tunneling microscopy (STM) is a powerful tool to explore the electronic structure of these nanoarchitectures with nanoscale resolution by correlating the measured dl/dV maps with the local electronic density of states.

However, Söde et al. found that the interpretation of STM experiments could misleadingly suggest electronic density confinement at the edges of uniform armchair graphene nanoribbons (GNRs), whereas theoretical predictions do not support the presence of intrinsically localized edge states. This deceptive confinement effect was attributed to a lack of cancellation between positive and negative regions of the wave function along the edges. Numerous subsequent studies have reported dl/dV data showing confinement of electronic density at the edges and pores of more complex geometries, yet there remains a lack of consensus on its interpretation.

In this work, researchers from DIPC in collaboration with researchers from the Technical University of Munich (TUM), Al-Azhar University and Kyoto University demonstrate that dl/dV mapping in carbon-based nanoarchitectures is influenced by a wave function decay effect that can result in a deceptive spatial distribution of electronic density. This effect is examined in semiconducting gulf-type GNRs and nanoporous graphene (NPG) structures synthesized on-surface, where dl/dV maps show the confinement of valence and conduction band states at the edges and nanopores of both structures. Density Functional Theory (DFT) calculations confirm that these measurements correspond to electronic states delocalized across the entire carbon nanoarchitecture, ruling out any intrinsic wave function localization. The deceptive confinement effect is explained by the faster decay of high-momentum Fourier components



On the left, atomic structure of a gulf-type GNR taken with atomic force microscopy (AFM), and the corresponding dl/dV map taken at positive bias voltage showing the confinement of conduction band states to the gulf-type edges. On the right, calculated conduction band state wave-function, which is delocalized over the entire GNR backbone, and the corresponding local density of states (LDOS) map simulation at realistic tip-sample distances, their spatial dependence being quite different. The LDOS map simulations account for the Fourier filtering effect and reproduce the experimental data.

### STM measurements are subject to a wave function decay into the vacuum that masks the undisturbed electronic orbital shape

of the wave function into the vacuum region above the sample. As the wave function decays to realistic tip-sample distances, only the lowest momentum Fourier components contribute to its spatial distribution, which appears localized at the edges and nanopores.

Although the decay of electronic orbitals into vacuum is a well-known effect observed in many surfaces and molecular assemblies, the unique edge and nanopore morphologies significantly influence the apparent orbital confinement in carbon-based nanoarchitectures. Thus, this work provides crucial understanding for the accurate interpretation of STM experiments and highlights the essential insights provided by theoretical calculations.



# Uncovering low-frequency vibrations in surface-enhanced Raman Scattering of organic molecules

Boehmke Amoruso A, Boto RA, Elliot E, de Nijs E, Esteban R, Foldes T, Aguilar-Galindo F, Rosta E, Aizpurua J, and Baumberg JJ 

Raman Scattering is a powerful spectroscopic technique to optically characterize molecules by interrogating their vibrational properties. When molecules are placed near the surface of metallic nanocavities that confine light into extremely small regions through plasmonic resonances, the resulting Surface-Enhanced Raman Spectroscopy (SERS) signal becomes enhanced, and thus sensitive to tiny amounts of analyte, and even to single molecules.

However, most of the research on SERS of organic molecules focuses on vibrations of relatively large energy, associated with the localized motion of a specific bondings involving two or three atoms within the molecule. Typical vibrational modes of this kind are, for instance, stretching or bending modes within pairs of atoms, which show scattering peaks at a particular wavevector values running from about 200  $cm^{-1}$  up to 3,000  $cm^{-1}$  in the Raman spectrum. These vibrations serve to identify the presence of a particular metabolite, or the occurrence of a specific chemical reaction.

A much less explored, and often elusive range of vibrational energies in the Raman spectrum occurs for wavevector excitation below 200 cm<sup>-1</sup>, reaching even a few tens of cm<sup>-1</sup> in the TeraHertz range (THz). These low-energy vibrational modes involve more complex motions along the molecule, often involving many atoms, or even collective motion along chains of molecules where the vibrational modes acquire a phonon-like propagating nature. To access this regime of low-energy vibrational excitation is very challenging experimentally, as these vibrational peaks are often masked by a strong emission background. The theoretical interpretation of the modes is equally challenging as the motion of several hundreds atoms in complex motions along molecular rings and chains, requires a considerable capacity of computation and classification.

In this work, researchers at DIPC and the Center for Materials Physics in San Sebastian, together with the Nanophotonics group at the University of Cambridge, analyze the low-energy vibrations of SERS spectra of seven canonical organic molecules forming self-assembled monolayers sandwiched in Nanoparticleon-a-Mirror (NPoM) plasmonic structures. By combining a careful experimental procedure to eliminate the strong low-energy background with quantum simulations of the low-energy vibrational modes that



Example of some of the low energy vibrations identified in the Raman spectra of molecules self-assembled in a nanocavity. The vibrational modes are associated with tapping/shearing motion of atoms along the molecule. A comparison of the vibrational modes as theoretically obtained with (top) and without (bottom) moleculemolecule interactions reveals the presence of collective phononic effects at these low energies along the self-assembly. The vibrations of the single molecules (marked by vertical lines in the bottom panel) split into multiple hybridized vibrations once the moleculemolecule interactions are included, providing a key ingredient to interpret SERS spectra at THz frequencies.

include the details of the chemical interaction between the molecules in the layer as well as with the metallic surface, the authors unveil and classify the main THz spectral features of such molecular assemblies. The results show that the low-energy vibrations are sensitive to molecule-molecule interactions and to the atomistic configuration with respect to the metallic surface, which could lead to improved characterization of molecule-metal interactions at the atomic scale. Furthermore, by exploiting the formation of metallic picocavities (atomic protrusions further localizing the electromagnetic field produced within the NPoM cavity), light is able to excite vibrations in only one or very few individual molecules of the whole assembly, and thus narrow SERS spectral features can be observed. This indicates that the broad THz lines observed in a typical SERS experiment can be largely attributed to inhomogeneous broadening and molecule-molecule interactions. The use of plasmonic nanocavities and picocavities could thus open a novel roadmap to access the elusive THz vibrations in SERS.



Low-energy vibrations in SERS at THz frequencies experimentally revealed and theoretically interpreted in state-of-the-art plasmonic nano- and pico-cavities

## On-chip phonon-enhanced IR near-field detection of molecular vibrations

Bylinkin A, Castilla S, Slipchenko TM, Domina K, Calavalle F, Pusapati V-V, Autore M, Casanova F, Hueso LE, Martin-Moreno L, Nikitin AY, Koppens FHL, and Hillenbrand R *Nature Communications* 15, 8907 (2024)

Molecules have some sort of fingerprints, unique features that can be used to differentiate them. Each type of molecule, when illuminated with the right light, vibrates at a characteristic frequency (its resonance frequency, which typically occurs at infrared frequencies) and strength. Similar to what can be done with human fingerprints, one can exploit this information to distinguish different types of molecules or gases from each other. That can also protect us from potential dangers, by identifying poisonous and dangerous substances or gases instead of criminals.

**One conventional approach is** infrared fingerprint spectroscopy, which uses infrared reflection or transmission spectra to identify different molecules. However, the small size of organic molecules compared to the infrared wavelength results in a weak scattering signal, making it challenging to detect small quantities of material. In recent years, this limitation has been addressed using Surface-Enhanced Infrared Absorption (SEIRA) spectroscopy. SEIRA spectroscopy leverages infrared near-field enhancement provided by rough metal surfaces or metallic nanostructure to amplify the molecular vibrational signals. The main advantage of SEIRA spectroscopy is its ability to measure and study minute material quantities.

Recently, phonon polaritons—coupled excitations of electromagnetic waves with atomic lattice vibrations—particularly hyperbolic phonon polaritons in thin layers of hexagonal boron nitride (h-BN), have emerged as promising candidates for boosting the sensitivity of SEIRA spectroscopy. Previously, we demonstrated that phonon polaritons can be applied for SEIRA spectroscopy of nanometer-thin molecular layers and gas sensing, thanks to their long lifetimes and ultra-high field confinement.

However, SEIRA spectroscopy remains a far-field technique that requires bulky equipment, such as light sources, SEIRA substrates, and typically nitrogen-cooled infrared detectors. This reliance on large instruments limits its potential for miniaturization and on-chip applications. In parallel, we have been investigating graphene-based infrared detectors that operate at room temperature, and we have shown that phonon polaritons can be electrically detected and can enhance detector sensitivity.

By combining these two progresses, a team of researchers has now successfully demonstrated the first on-chip phononic SEIRA detection of molecular vibrations. This result was made possible through the



Illustration of an on-chip molecular vibration sensor based on a graphene IR detector, where phonon polaritons (bright rays) enhance the molecular fingerprint signal encoded in the photocurrent.

# Graphene-based sensor reads molecular fingerprints through electric current at room temperature.

joint experimental efforts of CIC nanoGUNE and ICFO researchers, along with theoretical support from the groups of Dr. Alexey Nikitin at DIPC and Prof. Luis Martín-Moreno at the Instituto de Nanociencia y Materiales de Aragón (CSIC- Universidad de Zaragoza). The researchers employed ultra-confined HPhPs to detect molecular fingerprints in nanometer-thin molecular layers directly in the photocurrent of a graphene-based detector, eliminating the need for traditional bulky IR detectors.

One of the most exciting aspects of this approach is that this graphene-based detector opens the way towards miniaturization. By integrating this detector with microfluidic channels, we could create a true 'lab-on-a-chip', capable of identifying specific molecules in small liquid samples— paving the way for medical diagnostics and environmental monitoring.

In a longer-term picture, we believe that on-chip infrared detectors operating at room temperature could enable rapid molecular identification, potentially integrated into smartphones or wearable electronics. We further believes that this would offer a platform for compact sensitive, room-temperature infrared spectroscopy.



# Fluorescence imaging of individual ions and molecules in pressurized noble gases for barium tagging in <sup>136</sup>Xe

Byrnes NK, Dey E, Foss FW, Jones BJP, Madigan R, McDonald AD, Miller RL, Norman LR, Navarro KE, Nygren DR, and NEXT Collaboration

𝔗 Nature Communications 15, 10595 (2024)

The search for neutrinoless double beta decay  $(0\nu\beta\beta)$  remains one of the most important searches in particle physics, as its discovery would confirm the Majorana nature of neutrinos and might provide experimental basis to theories that can explain the asymmetry between matter and antimatter in the universe.

A promising avenue to enable a background-free search involves tagging the barium ion (Ba<sup>2+</sup>) produced in the decay of <sup>136</sup>Xe, together with the emission of two electrons. This technique is being pioneered by the NEXT collaboration and in this study the authors report the first demonstration of selective imaging of individual Ba<sup>2+</sup> ions at the gas-solid interface in a pressurized noble gas, achieving a crucial technological milestone for barium tagging.

Using molecular chemosensors specifically designed for  $Ba^{2+}$ , the researchers were able to detect fluorescence signals from single ions within 10 bar of xenon gas. The ions were resolved with a diffraction-limited optical system over a  $1 \times 1$  cm<sup>2</sup> scan area. This setting closely mimics the conditions that would be found in a future large-scale xenon gas detector. The ability to image individual ions under these conditions represents a major step forward, overcoming challenges such as maintaining optical resolution and suppressing background signals in dense gases.

This achievement significantly strengthens the feasibility of background-free  $0\nu\beta\beta$  searches. Additionally, the microscopy platform developed for this experiment opens a new window into the photophysics of fluorescent molecules and chemosensors at the solid-gas interface.

The system can be implemented within the pressure vessel of a time projection chamber such the one of the NEXT experiment with only small modifications. As such, this result advances the technology available for  $0\nu\beta\beta$  experiments and introduces a powerful method for studying single-molecule phenomena under conditions previously inaccessible. Imaging single Ba<sup>2+</sup> ions in xenon represents a critical step toward realization of a background-free, ton-to-multi-ton scale  $0\nu\beta\beta$  experiment based on barium tagging.



Large scale raw data image of BODIPY molecules drip-coated onto a slide surface. The image is resolved with point-spread function close to the Abbe Diffraction Limit. Bright points consistent with single molecule fluorescence are observed over a scan region of 1 mm<sup>2</sup>.

Single Ba<sup>2+</sup> ions have been imaged in high pressure xenon gas using turn-on fluorophores, representing the first demonstration of imaging of individual Ba<sup>2+</sup> ions within a candidate active medium of a time projection chamber for  $0\nu\beta\beta$ 



Image of a slide spin-coated in IPG-1 chemosensor, showing the activity with (right) and without (left) added  $Ba^{2+}$ .



# A deep learning method that identifies cellular heterogeneity using nanoscale nuclear features

Carnevali D, Zhong L, González-Almela E, Viana C, Rotkevich M, Wang A, Franco-Barranco D, Gonzalez-Marfil A, Neguembor MV, Castells-Garcia A, Arganda-Carreras I, and Pia Cosma M 𝔗 Nature Machine Intelligence 6, 1021 (2024)

Technology paves the way for new diagnostic and monitoring strategies for disease by capturing and scanning images of cells. The tool, AINU (AI of the NUcleus), scans high-resolution images of cells.

The images are obtained with a special microscopy technique called STORM, which creates a picture that captures many finer details than what regular microscopes can see. The high-definition snapshots reveal structures at nanoscale resolution. The AI can detect rearrangements inside cells as small as 20 nm, or 5,000 times smaller than the width of a human hair. These alterations are too small and subtle for human observers to find with traditional methods alone.

AINU is a convolutional neural network (CNN), the same type of AI behind facial recognition and selfdriving car vision. In medicine, CNNs help detect signs of disease in images like mammograms or MRIs. AINU uses this visual intelligence to analyze how cellular components are arranged in 3D, especially within the nucleus.

Researchers trained AINU using nanoscale images of many different cells. The AI learned to distinguish between normal and cancerous cells based on nuclear features like DNA organization or enzyme distribution. It also spotted early signs of infection by herpes simplex virus type-1 – detecting changes just one hour after infection, long before symptoms appear.

Our method sees microscopic nuclear changes immediately after a virus enters. This could help in diagnosing infections faster, or in designing better treatments and vaccines.

The ultimate goal is to use AINU clinically, allowing doctors to detect disease or infection from simple blood or tissue samples. However, current STORM imaging is only available in specialized labs, and it captures only a few cells per scan. Clinical applications would require broader imaging and more accessible equipment.

Despite these hurdles, AINU is already proving valuable in research. It accurately identifies pluripotent stem cells–cells that can become any other cell type – without relying on animal testing. AINU offers a faster, more ethical way to spot high-quality stem cells, helping make therapies safer.

This technology could one day personalize treatments and improve outcomes. With such precise information, we hope to give doctors a head start in diagnosing and treating disease.



Very high resolution image of a HeLa cancer cell used to train AINU.

Our method can detect cells that have been infected by a virus very soon after infection begins



# Efficient near-infrared organic light-emitting diodes with emission from spin doublet excitons

Cho HH, Gorgon S, Londi G, Giannini S, Cho C, Ghosh P, Tonnelé C, Casanova D, Olivier Y, Baikie TK, Li F, Beljonne D, Greenham NC, Friend RH, and Evans EW *⊗* Nature Photonics 18, 905–912 (2024)

The development of luminescent organic radicals has resulted in materials with excellent optical properties for near-infrared (NIR) emission. Light generation in this range could be used for organic light-emitting diodes (OLEDs), as well as healthcare diagnosis and treatment to surveillance, communications and other security applications.

Although an external quantum efficiency greater than 20% in electroluminescence has been demonstrated for visible-light OLEDs, and commercial displays are commonplace, the performance of NIR OLEDs is generally limited to 5% external quantum efficiency using fully organic emitters with emission peak wavelengths at 800 nm and longer. The materials approach and mechanisms for efficient visiblelight OLEDs by maximizing luminescence from singlet and triplet excitons have not translated to efficient NIR OLEDs.

Doublet fluorescence from organic radicals is an emerging basis for the development of highly efficient NIR light-emitting devices that exploit favorable optical, electronic and spin properties. Almost 100% internal quantum efficiency for electroluminescence was demonstrated in radical OLEDs exploiting tris(2,4,6-trichlorophenyl)methyl (TTM)-based radicals. This performance shows that using radical emitters with spin-allowed doublet emission is a conceptually superior solution to elegantly circumvent the spin statistics limited efficiency issue inherent to conventional closed-shell organic materials (25% internal quantum efficiency).

Although the unpaired electron arrangements of radicals enable efficient radiative transitions within the doublet-spin manifold in organic light-emitting diodes, their performance is limited by non-radiative pathways introduced in electroluminescence.

Now, a team of researchers uses a host-quest design for organic light-emitting diodes that exploits energy transfer with a boost of external quantum efficiency for 800 nm emission. The tris(2,4,6-trichlorophenyl)methyl-triphenyl-amine (TTM-TPA) radical guest is energy-matched to the triplet state in a chargetransporting anthracene-derivative (MADN) host.



Schematic illustration of intersystem dual energy transfer between host MADN and radical TTM-TPA in doublet electroluminescence devices.

Spin-allowed energy transfer and state matching drive efficient delayed emission, offering a pathway to minimize non-radiative losses in NIR devices

The researchers show from optical spectroscopy and quantum-chemical modelling that reversible hostguest triplet-doublet energy transfer allows efficient harvesting of host triplet excitons. The luminescent NIR radical system is implemented in high-performing OLEDs with a maximum external quantum efficiency of 9.6% for electroluminescence at 800 nm that operate to the high maximum radiance of  $\sim$ 68,000 mW sr<sup>-1</sup> m<sup>-2</sup>, with low efficiency roll-off and enhanced stability. This new design boosts performance in radical-based OLEDs and has broad implications for reducing non-radiative losses in devices beyond light-emitting applications with NIR light.



# Bending rigidity, sound propagation and ripples in flat graphene

Aseginolaza U, Diego J, Cea T, Bianco R, Monacelli L, Libbi F, Calandra M, Bergara A, Mauri F, and Errea I **A** Nature Physics 20, 1288 (2024)

Understanding why 2D materials are stable remains in some ways unsolved. This paper, led by the Quantum Theory of Materials group at CFM, with the participation of DIPC associates, brings together various factors that are important – symmetry and anharmonicity – and combines them to propose a resolution to this long-standing puzzle.

This study addresses a longstanding puzzle in the mechanical understanding of graphene and all twodimensional (2D) materials: how out-of-plane flexural vibrations (bending modes) behave and how they affect physical properties like sound propagation and bending rigidity. The core finding is that rotational symmetry protects the quadratic dispersion of these flexural modes, even when accounting for anharmonic phonon-phonon interactions. This makes the bending rigidity non-divergent, challenging previous theories.

In the standard harmonic approximation, flexural vibrations in graphene are predicted to have a guadratic dispersion. However, this leads to the unphysical result that in-plane acoustic waves cannot propagate sound, prompting some to argue that interactions between phonons must linearize the dispersion. While this explanation permits sound propagation, it leads to a paradox: the bending rigidity becomes dependent on the system size, suggesting it diverges - an unsatisfactory outcome for a material known for its remarkable strength.

The authors propose a resolution based on a symmetry principle. Both harmonic and anharmonic phonons are derived from second derivatives of energy functions – the potential energy in the harmonic case and the full free energy in the anharmonic case - both of which are rotationally invariant. This symmetry requires that the dispersion of flexural modes remains quadratic even with anharmonic interactions.

The theory was tested using atomistic simulations and membrane models, and both confirmed that the guadratic nature of the flexural modes is preserved. Importantly, while a guadratic dispersion in the harmonic theory prevented sound propagation, in the anharmonic framework sound still propagates as it has to.

One major implication is that the bending rigidity remains finite, regardless of the system size overturning the common assumption that it diverges due to linearized flexural modes.



The amplitude of ripples in a membrane are typically studied via the height correlation function in momentum space,  $\langle |h_{q}|^{2} \rangle$ . Here, the height fluctuations of graphene are presented from the Fourier transform of the height-height correlation function, versus the wave number q, at 12.5 K. When there is the full rotational invariance (RI), the physical result scales as  $q^{-4}$  in the classical regime; but the exponent is lower when rotational invariance is broken (no RI). The physical RI results coincides practically with the harmonic solution. Bending rigidity scales as the correlation function times q<sup>4</sup> and so diverges in the absence of rotational symmetry, though not when rotational symmetry holds.

This paper addresses the long-standing puzzle of 2D material stability by unifying key factors such as symmetry and anharmonicity into a proposed resolution

While these results significantly improve our understanding of 2D materials' mechanical behavior, they apply only to ideal, unstrained, flat systems. In real-world applications, substrates or external strains might break rotational symmetry, altering such behavior. Future work will investigate whether static ripples naturally form in unstrained graphene and if their formation is energetically favorable.

Ultimately, this work provides a new, symmetry-based framework for understanding thermal and mechanical properties of all 2D materials like graphene.

# Detection of a universal core-halo transition in dwarf galaxies as predicted by Bose-Einstein dark matter

Pozo A, Broadhurst T, de Martino I, Chiueh T, Smoot GF, Bonoli S, and Angulo R & Physical Review D 110, 043534 (2024)

In this work, we analyze stellar profiles and velocity dispersions of a representative sample of dwarf galaxies, including both Milky Way satellites and isolated Local Group members. We find that all these systems exhibit a clear core-halo structure, with a pronounced transition in density at a radius of approximately 1 kpc.

Such a structure is unexpected in the standard CDM paradigm, which predicts cuspy, concentrated density profiles with no inherent transition. Instead, the observed profiles align remarkably well with the predictions of Bose-Einstein condensate dark matter ( $\psi$ DM), a model where dark matter behaves as a coherent wave.  $\psi$ DM naturally forms a dense central soliton core surrounded by a diffuse halo generated by wave interference patterns.

We show that the observed stellar density profiles are well fit by the  $\psi$ DM core-halo structure, with only one free parameter: the boson mass. Additionally, we find that the measured velocity dispersions in these galaxies peak at the core radius and decline outward-again, consistent with the  $\psi$ DM prediction. This agreement supports a boson mass of approximately  $1.5 \times 10^{-22}$  eV, in line with independent dynamical modeling.

These findings suggest that stars in these dark-matter-dominated galaxies trace the underlying wave structure of a guantum dark matter field. Light bosonic particles, such as axions predicted by string theory, provide a compelling alternative to heavy particle dark matter in explaining the structure and kinematics of dwarf galaxies.

Our results provide observational support for  $\psi$ DM and reinforce the idea that core-halo transitions are not exceptional features, but rather a generic signature of wave dark matter dynamics.



Stellar profiles of Local Group dwarfs, rescaled by their transition radius, reveal a common core-halo structure, with orbiting dwarfs showing more pronounced gaps correlated with their pericenter distance from the Milky Way.



A common core-halo structure is observed in dwarf galaxies, with a sharp density transition near 1 kpc



profiles that fit the observed stellar halo slopes of the isolated and orbiting dwarfs, respectively.



Isolated Dwarf Galaxies: This figure shows the star count profiles versus dwarf galaxy radius for the well studied "isolated" dwarf galaxies in the local group, lying outside the virial radius of the Milky Way. (In the right panels D<sup>-</sup> shows the distance from the Milky Way galaxy center.) Each dwarf galaxy has an extended halo of stars stretching to ~2 kpc and most evident on the linear scale of right hand panel. Cores are also evident on a scale <1 kpc in each dwarf. A standard Plummer profile (red curve) is seen to fit approximately the core region but falls well short at large radius. Our predictions for light boson dark matter,  $\psi DM$ , are shown in green, where the distinctive soliton profile provides an excellent fit to the observed cores with the surrounded halo of excited states that average azimuthally to an approximately NFW-like profile beyond the soliton radius. The observed cores are in excellent agreement with the predicted soliton, best seen on a log scale in the left panels, and the predicted  $\psi$ DM halo (grey curve) is also seen to match well the observed halos, including the characteristic density.

The left hand panel compares all the dwarf profiles scaled ( $\Sigma_{0*}$  = 1000 M /Kpc<sup>-2</sup>) and all the core radii set to 0.3 kpc. The profiles are very similar in the core region, differing in the extended halo region relative to the core, with the isolated galaxies (bluer colors) having denser halos than the orbiting dwarfs (redder colors). The right hand panel shows the projected simulation profiles for  $\psi$ DM by Schive, Chiueh & Broadhurst (2020), where little dependence on the degree of tidal stripping is predicted for the core region, in contrast to the halo region bracketed in grey where stripping is significant. The duration of stripping is indicated by the legend and also shown in the inset of the left hand panel spanning 1-4 Gyrs, and matching well the observed range of halo profiles. Note, the simulations predict the halo slope is relatively shallow and fairly independent of the degree of stripping, in good agreement with the mean halo profile of the isolated dwarfs (averages of the normalized profiles shown in the left panel, blue data) and the orbiting dwarfs (red data points), including the larger corehalo transition of the orbiting dwarfs. The NFW profile fits to the halos are also shown and can be seen to fall well below the prominent cores. These last two (orange and grey lines) are examples of the required pure NFW

# Indistinguishability of identical bosons from a quantum information theory perspective

Englbrecht M, Kraft T, Dittel C, Buchleitner A, Giedke G, and Kraus B *Physical Review Letters 132*, 050201 (2024)

Fundamentally, all identical particles are indistinguishable. This has profound consequences for the properties of many-body systems and plays a crucial role for certain bosonic quantum computing approaches such as boson sampling or the KLM scheme that are based on letting many photons interfere in a multi-mode interferometer and only measure the photon number in the output modes.

In practice, not all degrees of freedom of the bosons can be perfectly controlled (e.g., due to time jitter or frequency fluctuations of the photon source). This raises the question how good a given state of N bosons is and to judge the quality of a many-boson state or the source that produces it. A practically relevant question is whether these bosons behave indistinguishably if they coincide in all accessible degrees of freedom or not because of other, inaccessible degrees of freedom that distinguish them.

This paper develops a general way to quantify how indistinguishable identical bosons are in quantum experiments involving linear optics. Using ideas from quantum information theory, the authors define a measurable quantity  $p_{N}$ , the expectation value of the projector on the symmetric N-particle subspace, that captures how "boson-like" the particles are, even when they may have hidden differences. This generalizes and unifies previous definitions of many-particle indistinguishability. However, like all these guantities, for large particle number  $p_N$  is exponentially difficult to measure or compute. But the authors derive a lower bound in terms of a two-particle indistinguishability measurement, that can be efficiently obtained and that provides a tight bound for highly indistinguishable states. Additionally, the authors show that the measurements enabled by the interferometric setting are tomographically complete (that is, they allow to distinguish all states that are distinct in terms of their accessible degrees of freedom) and introduce a compatible notion of what it means for states to describe perfectly distinguishable bosons and show that the set of these states is not convex



this process depends on how indistinguishable the input photons are.

For many photons and modes, p<sub>N</sub> is exponentially hard to compute or measure. But it can be bounded from below using the two-particle indistinguishability p<sub>2</sub>.



States of many indistinguishable photons are a resource for guantum computation. Here we derive a general method to guantify how indistinguishable the photons are



Boson sampling experiments and linear-optics quantum computing send a large number of photons through an interferometer and measure the particle number in the output ports. The difficulty of classically simulating

# Universal features of entanglement entropy in the honeycomb Hubbard model

D'Emidio J, Orus R, Laflorencie N, and de Juan F & Physical Review Letters 132, 076502 (2024)

Entanglement entropy is a measure of the degree of quantum entanglement between two subsystems constituting a two-part composite quantum system. But entanglement entropy also guantifies the information shared between a subsystem and its environment in a guantum manybody wavefunction.

Interestingly, the finite-size scaling form of entanglement entropy has contributions that depend uniquely on universal physical quantities, making it a powerful probe to characterize strongly correlated systems. A widely known example of this is found in one-dimensional critical systems, where entanglement entropy grows logarithmically in the subsystem size with a prefactor given by the central charge.

In two dimensions, things get more complicated. On one hand, the leading term of the entanglement entropy grows at most proportionally with the boundary of the subsystem, the so-called "area law". On the other, if the subsystem contains sharp corners, critical ground states display a subleading universal logarithmic contribution.

Despite a wide variety of numerical work investigating spin and boson systems, the universal features of entanglement entropy of two-dimensional interacting fermions have remained, for the most part, an unexplored frontier. The pioneering work of Grover introduced auxiliary-field determinental quantum Monte Carlo (DQMC) simulations as a promising route to large-scale calculations of the Rényi entanglement entropy of interacting fermions. But the sampling from uncorrelated replica configurations make the estimator suffer from rare events that dominate the statistical average. Consequently, the universal features of entanglement entropy in 2D have remained out of reach for these methods.

Now, a team of researchers presents an improved method to compute the Rényi entanglement entropy in DQMC that solves the above mentioned sampling problem and enables unprecedented precision. To do so, the team develops an improved equilibrium method for DQMC simulations.

The approach harnesses the power of importance sampling by introducing an extended ensemble of Monte Carlo configurations in which the entangling region is allowed to fluctuate. Remarkably, the original Grover's formulation admits such an extended ensemble that can be simulated efficiently using standard DQMC techniques. To demonstrate the power of this technique, the scientists use it to study a benchmark system, a classic model of interacting fermions in two dimensions, the half-filled honeycomb Hubbard model at T = 0. Doing so, they detect, for the first time, logarithmic corrections to the area law in a 2D model of interacting fermions. Importantly, they find that such logarithmic terms can be sensitive to the type of entanglement cut that is used.



Entanglement entropy for the honeycomb Hubbard model as a function of interaction strength. The inset shows the fluctuating entangling region used to compute the entanglement entropy.



strength U in a triangle geometry. The method extracts for the first time the corner subleading logarithmic corrections and shows their interaction dependence, peaking at the critical point U=3.8.

computes subleading logarithmic corrections to entanglement effects through entanglement



# A new Quantum Monte Carlo method exploiting importance sampling entropy, opening the way to a reliable path to probe guantum critical

# Evolution of superconductivity in twisted graphene multilayers

Long M, Jimeno-Pozo A, Sainz-Cruz H, Pantaleon PA, and Guinea F. Proceedings of the National Academy of Sciences 121, e2405259121 (2024)

Superconductivity, the phenomenon where electrical current flows without resistance, holds promise for revolutionizing technologies, from power grids to magnetic levitation. This study delves into the intriguing world of graphene based superconductors, shedding light on how twisting multiple layers of graphene can influence their superconducting properties.

The angle at which graphene layers are twisted plays a pivotal role in determining their electronic properties. When layers are misaligned by a "magic angle" of approximately 1.1 degrees, the electronic interactions between the layers create a unique energy landscape. This configuration leads to the formation of "moiré patterns", large-scale interference patterns that significantly alter the material's electronic behavior. In twisted bilayer graphene, these moiré patterns have been linked to the emergence of superconductivity and other correlated electronic phases.

Building upon the insights from twisted bilayer graphene, this study is focused on "twisted double bilayer graphene" and "helical trilayer graphene." In twisted double bilayer graphene, two bilayer graphene sheets are stacked with a twist, while helical trilayer graphene consists of three layers twisted in a specific sequence. These configurations introduce new complexities and opportunities in understanding superconductivity.

The researchers employed advanced theoretical models to analyze how long-range charge fluctuations -variations in the distribution of electric charge over distances- affect superconductivity in these multilayer graphene systems. Their findings reveal that the critical temperature and the order parameter differ significantly between twisted double bilayers and helical trilayers on one hand, and twisted bilayer graphene on the other. The temperature at which a material becomes superconducting, known as the critical temperature, differs significantly between the systems studied. Twisted double bilayer and helical trilayer graphene exhibit distinct critical temperatures compared to twisted bilayer graphene, suggesting that adding more layers and varying twist angles can tune the superconducting properties. The order parameter is a measure that describes the state of the superconducting phase. Variations in this parameter among the different graphene configurations indicate that the nature of the superconducting state changes with the number of layers and their arrangement.

The study highlights the role of moiré Umklapp processes, interactions where electrons scatter in a manner influenced by the moiré pattern. These processes differ between the systems, contributing to the observed variations in superconducting behavior.



Understanding how twisting and layering graphene affects its superconducting properties is more than an academic pursuit; it has practical implications for developing advanced materials and technologies. By manipulating the twist angles and stacking sequences, scientists can engineer graphene-based materials with tailored superconducting characteristics, potentially leading to more efficient energy transmission, novel electronic devices, and guantum computing components.



# Catalog of topological phonon materials

Xu Y, Vergniory MG, Ma DS, Mañes JL, Song ZD, Bernevig BA, Regnault N, and Elcoro L Science 384, eadf8458 (2024)

The spectrum of phonons – essentially the energy as a function of momentum – and their wave functions, which represent their probability distribution in real space, can be computed using ab initio first principle codes. However, these calculations have so far lacked a unifying principle. For the quantum behavior of electrons, topology -a branch of mathematics- has successfully classified the electronic bands in materials. Can topology also characterize phonons?

In this article we uncovered that a wide range of materials could host topological phonons. We first computed the phonon bands of thousands of guantum materials, identifying their wavefunctions and characterizing them by their symmetries, which provide a sort of local structure of the phonons. After completing this step, we employed topology to classify the global behavior of the phonon bands.

Several phonon structure databases have been meticulously analyzed, revealing that at least half of the materials exhibit at least one non-atomic cumulative phononic band set. The team employed a formalism similar to that developed for characterizing electronic bands, as outlined in their previous work on Topological Quantum Chemistry (TQC).

Phonon offer a new avenue for achieving nontrivial band topologies in solid-state materials, potentially leading to phonon surface states that could complement or enhance electronic surface states. The robustness of the topological surface phonon states can be leveraged for applications like frequency filtering or mechanical energy attenuation under imperfect conditions, as well as for heat transfer and infrared photoelectronics. Topological phonons could also pave the way for creating phonon diodes or acoustic waveguides. Analyzing data from over ten thousand materials, gathered from ab-initio calculations and stored in databases like PhononDB@kyoto-u and the Materials Project, we found that 50% of materials exhibit at least one non-trivial gap.

We discovered more topological structures in phonons than we initially expected, and we anticipate that topological phonons will lead to rich and unconventional physics, much like topological electrons have. We emphasized the importance of validating predictions for materials hosting topological phonons, noting that such experiments might be more challenging than those for electronic topology, due to lack of direct imaging techniques. The phonons have been cataloged in a public repository (https://www. topologicalquantumchemistry.com/topophonons), where researchers can access specific materials. Every phononic surface state is listed in this database; the next step would be for experimentalists to measure them.

The team envisions new physics that may emerge from the coupling between topological electrons and phonons. If topological electron surface states coexist with phononic ones, this could facilitate strong electron-phonon coupling on the surface -though potentially not in the bulk- potentially leading to surface superconductivity.



We have discovered more topological structures in phonons than we initially expected, and we anticipate that topological phonons will lead to rich and unconventional physics, much like topological electrons


# Morphological sensitivity to pH of silica and chalk nanocrystalline self-organized biomorphs

Menichetti A, Manzi J, Otálora F, Montalti M, and García-Ruiz JM **S** Small Science 4, 2400090 (2024)

The bottom-up design of hierarchically organized nanostructures is a powerful strategy for achieving new materials with innovative functionalities. Biomorphs consist of thousands of carbonate nanocrystals aligned through silica-induced interactions, forming curved, noncrystallographic, and hierarchically textured structures. Their formation is considered an autocatalytic process driven by the inverse pH solubility of alkaline-earth carbonates and silica. As carbonate crystals form, the pH drops due to carbonate removal, which triggers silica precipitation. This, in turn, raises the pH again, initiating further carbonate nucleation and sustaining the coprecipitation cycle. The morphology and texture of biomorphs can be controlled by adjusting local conditions, namely temperature, pCO<sub>2</sub>, and pH.

A pioneering study of the spatial and temporal evolution of pH inside silica gels during the precipitation of witherite biomorphs correlated pH with a photographic record of the spatial and temporal evolution of the morphologies of the aggregates. The work demonstrated that understanding the role of pH in morphogenesis requires measuring the pH locally in real-time using a non-invasive technique.

Now, a team of DIPC and University of Bologna researchers has developed a technique utilizing fluorescence imaging to detect pH on the growing front of biomorph in solution, reporting evidence of oscillations in the local pH at the front. The new ratiometric approach employs a probe that can be excited at two different wavelengths, producing two distinct fluorescence signals with varying pH dependencies. The ratio of the two signals remains independent of the local probe concentration and can be used to calculate pH.

This methodology eliminated artifacts in the pH measurements caused by probe concentration inhomogeneity due to diffusion, transport, photobleaching, or chemical degradation in the harsh alkaline conditions of the silica gel. The researchers demonstrate the use of the ratiometric fluorescent pH chemosensor to measure the variation of pH over time and across the silica gel during the growth of barium carbonate biomorphs. Changes in local pH were correlated with nucleation and biomorphic growth by combining optical transmission with fluorescence imaging.

The team measured the variation of pH in situ during a counter-diffusion precipitation experiment that formed barium carbonate biomorphs and compared it with a computer simulation of the growth



Precipitation simulations and in-situ noninvasive optical methods reveal pH's temporal and spatial evolution during biomorph morphogenesis.

found in natural biominerals

experiment under identical starting conditions. The results demonstrate the envisaged existence of only two pH-dependent regimes in the formation of biomorphs: fractal growth and biomorphic growth.

Interestingly, the morphogenetic process controlling the complex shaping of biomorphs is independent of silica speciation. This indicates that while pH (and subsequently silica species) has a substantial effect on the transition from fractal to biomorphic growth, the morphogenetic mechanism responsible for different biomorphic shapes is independent of pH and must be inherent to the propagation of the growth front.



## Biomorphs are silica-carbonate curved architectures with hierarchical textures reminiscent of structural principles

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## 538 Ab initio study of the influence of spin and orbital magnetic moments on the stability of magnetic and charge distribution in Co:ZnO monolayer

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## 540 Dynamics of vortex matter in 2D gapless superconducting materials with impurities

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## 541 Spin mixing in intramolecular singlet fission: a first-principles-based quantum dynamical study Kathir RK, Coto PB, and Thoss M. The Journal of Physical Chemistry Letters 15, 11517 (2024).

## 542 Time-resolved chemical bonding structure evolution by direct-dynamics chemical simulations Piris M, Lopez X, and Ugalde JM. The Journal of Physical Chemistry Letters 15, 12138 (2024).

## 543 Ion migration at metal halide perovskite grain boundaries elucidated with a machine learning force field

Samatov MR, Liu D, Zhao L, Kazakova EA, Abrameshin DA, Das A, Vasenko AS, and Prezhdo OV. The Journal of Physical Chemistry Letters 15, 12362 (2024).

## Marin-Villa P, Gaboardi M, Joseph B, Alabarse F, Armstrong J, Druzbicki K, and Fernandez-Alonso F. The Journal of Physical Chemistry Letters 16, 184 (2024).

## 545 Schottky defects suppress nonradiative recombination in CH<sub>3</sub>NH<sub>3</sub>Pbl<sub>3</sub> through charge localization

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## 546 On the parallelization of multipacting simulation codes for the design of particle accelerator components

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122 DIPC 2024

544 Methylammonium lead iodide across physical space: phase boundaries and structural collapse



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

DIPC Associates..... Ikerbasque Research Professors...... Distinguished Researchers..... Ikerbasque Research Associates ..... Ikerbasque Research Fellows..... Fellows ..... Postdoctoral Positions ..... Research Collaborators ..... PhD Students..... Research Assistants..... Engineers..... Technical Assistants..... Internships..... Undergraduate Candidates..... Master's Degree Student ..... Special Assignments ..... Gender Equality Committee......

# Researchers

## **DIPC** Associates

Maite Alducin Ochoa CSIC Ignacio Arganda-Carreras UPV/EHU Andrés Arnau Pino UPV/EHU Emilio Artacho Cortés CIC nanoGUNE Andrés Ayuela Fernández CSIC Rolindes Balda de la Cruz UPV/EHU Sara Barja Martínez UPV/EHU Aitor Bergara Jauregi UPV/EHU Sebastian Bergeret CSIC María Blanco Rey UPV/EHU Pedro Braña Coto CSIC Tom J. Broadhurst UPV/EHU Igor Campillo Santos Euskampus Daniele Cangialosi CSIC Silvina Cerveny CSIC Aurelia Chenu UNI.LU Deung-Jang Choi MPC Martina Corso CSIC Fernando Cossio Mora UPV/EHU David De Sancho Sánchez UPV/EHU Nuno De Sousa Teixeira Simia Technologies Adolfo Del Campo Echevarría UNI.LU Asier Eiguren Goyenetxea UPV/EHU Ion Errea López UPV/EHU Rubén Esteban Llorente CSIC Francesca Ferlaino LFUI Joaquín Fernández Rossier UPV/EHU Felix Fernández Alonso CFM Elena Formoso Estensoro UPV/EHU Daniel Franco Barranco University of Cambridge Idoia García de Gurtubay Gálligo UPV/EHU Dimas García de Oteyza Felderman CINN-CSIC-UNIOVI-PA Vitaly Golovach CFM Elton Gomes Dos Santos UoE Miguel Ángel Gosálvez Ayuso UPV/EHU Marek Grzelczak CSIC

Julen Ibáñez Azpiroz CFM Elisa Jiménez-Izal UPV/EHU Iñaki Juaristi Oliden UPV/EHU Stefan Kurth UPV/FHU Aritz Leonardo Lizeranzu UPV/EHU Xabier López Pestaña UPV/EHU Nicolás Lorente Palacios CSIC Jon Mattin Matxain Beraza UPV/EHU José María Mercero Larraza UPV/EHU Salvador Miret Artés IFF-CSIC Gabriel Molina Terriza MPC Álvaro Moreno Bergareche UPV/EHU Ángel Moreno Segurado CSIC Enrique Ortega Conejero UPV/EHU Mikhail Otrokov CFM José Ignacio Pascual Chico CIC nanoGUNE Juan Ignacio Pérez Iglesias UPV/EHU José María Pitarke De la Torre UPV/EHU Yuri Rakovich UPV/EHU Daniel Reta Mañeru UPV/EHU Elixabete Rezabal Astigarraga UPV/EHU Enrique Rico Ortega UPV/EHU Alberto Rivacoba Otxoa UPV/EHU Celia Rogero Blanco CSIC Jorge Sánchez Dolado CSIC Daniel Sánchez Portal CSIC Ane Sarasola Iñiguez UPV/EHU Frederik Schiller CSIC Gustavo Schwartz CSIC Ivo Souza UPV/EHU Eugene Tchulkov Savkin UPV/EHU Ilva Tokatly UPV/EHU Miguel Torrent Sucarrat UPV/EHU Geza Toth UPV/EHU Jesús Ugalde Uribe-Etxebarria UPV/EHU Lucía Vitali UPV/EHU Nerea Zabala Unzalu 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, Coulomb 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 Vyalikh

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.

## 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**

Ronen Zangi 01/02/2023–Present Computer simulations of biological and chemical systems. Statistical mechanics of finite systems.

Miguel Moreno Ugeda 15/06/2023–Present Low-temperature scanning tunneling microscopy and spectroscopy of two-dimensional materials and nanostructures.

Javier Aizpurua Iriazabal 01/12/2023–Present Theory of nanophotonics.

Paola Ferrario 01/01–15/09/2024 Neutrino physics.

Arantzazu García Lekue 01/01/2024–Present Modeling electron transport at the nanoscale. Theoretical investigation of electron processes at nanostructured surface.

Juan Manuel García Ruiz 01/01/2024–Present Crystallography and crystal growth.

Eduard Matito Gras 01/01/2024–Present Development of electronic structure methods and real-space descriptors of chemical bonding and aromaticity.

Konstantin Bliokh 01/05/2024–Present Complex classical and quantum waves.

## 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.

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 guantum interfaces.

Maia García Vergniory 01/01/2023–Present Prediction of new topological phases and materials. Daniel Rubén Zerzión 01/03/2023–Present Development and construction of the XeESS detector. Neutrino physics at the ESS.

Francesca Ferlaino 01/10/2024–Present Quantum Science Lab

## Ikerbasque Research Associates

Alexey Nikitin 01/01/2018–31/12/2024 Nanophotonics of 2D materials.

Raúl Esteban Angulo de la Fuente 01/06/2018–31/12/2024 Numerical simulations in cosmology.

David Casanova Casas 01/07/2018–31/12/2024 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.

## 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.

## Silvia Bonoli

01/09/2023–Present Formation and evolution of supermassive black holes in a cosmological context, combining theoretical models and observational data.

## Fernando de Juan Sanz 01/09/2023–Present

Topology and electronic correlations in quantum materials.

## Aitzol García Etxarri

01/11/2024–Present Nanophotonics theory.

## **Ikerbasque Research Fellows**

Fellows

Aitzol García Etxarri 01/11/2019-31/10/2024 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.

Tobias Daniel Grass 01/10/2022-Present Quantum simulation and synthetic quantum matter.

Claire Tonnelé 01/09/2023-Present Electronic structure in molecular photophysics and optoelectronics.

Stefano Roberto Soleti 01/09/2024-Present Neutrinoless double beta decay with the NEXT experiment.

María Navarro Gastiasoro 01/01/2023-Present Exotic superconductivity and correlation in quantum materials.

Helena Almazán Molina 15/09/2024-Present Neutrino physics in NEXT and WCTE experiments.

## Postdoctoral Positions

Jens Oliver Stücker 02/09/2019-31/08/2024 Cosmology.

Tao Wang 07/10/2019-31/01/2024 On-surface synthesis of functional molecular materials.

Rubén Rodríguez Ferradás 01/05/2020-20/08/2024 Development of new density functional approximations.

Jonathan D'Emidio 05/10/2020-28/08/2024 Quantum Monte Carlo calculations and networks of tensors.

Rafael Ramis Cortés 08/02/2021-29/02/2024 Molecular dynamics of potassium channels.

María Jesús Morán Plata 20/09/2021-30/11/2024 Catalysis toward platinum substrates for drug delivery.

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

Ricardo Ortiz Cano 16/10/2021-29/02/2024 Quantum correlations in graphene-based nanostructures.

Valerio Di Lisio 15/11/2021-14/11/2024 Non-equilibrium dynamics of amorphous polymers and other materials.

Rodrigo Voivodic 06/12/2021-Present Cosmology – Large scale structure.

lñigo Robredo Magro 01/02/2022-30/06/2024 Topological quantum materials as platforms for quantum computers.

Jorge Humberto Melillo 07/02/2022-06/02/2024 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 01/03/2022-28/10/2024 Quantum technologies - Quantum metasurfaces.

Beatriz Robles Hernández 01/03/2022-29/02/2024 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.

Luis Alejandro Miccio Stefancik 01/04/2022-14/01/2024 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.

Anastasija Skurativska 11/07/2022-10/07/2024 Quantum technologies - Quantum annealing hardware-based on non-conventional superconducting circuitsand new quantum materials.

Haoyu Hu 22/09/2022-18/11/2024 Development of flat band theory methods for search of new materials.

Stefano Roberto Soleti 26/09/2022-31/08/2024 Neutrinoless double beta decay with the NEXT experiment.

Raphael Enoque De Paiva 30/09/2022-Present Development of photoactivatable anticancer metal complexes and nanomaterials. 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.

Ana Cristina Carrasco Gento 01/01/2023-Present Bioorthogonal photocatalysis towards metal substrates.

Ricardo Rama Eiroa 16/01/2023-Present Designing the next generation of hard-drives using two-dimensional materials.

Jose Eduardo Barcelon 23/01/2023-Present On-surface trapping of Ba ions by functionalized surfaces.

Fei Gao 23/01/2023-Present Hybrid graphene nanoarchitectures for electrochemical sensing.

Raúl Guerrero Avilés 01/04/2023-14/06/2024 Adsorbing atoms and molecules on van der Waals heterostructures.

Charles Mark Lewis 01/04/2023-Present Neutrino physics as part of ESSCEvNS.

Mesías Agustín Orozco Ic 05/04/2023-30/09/2024 Theoretical physical chemistry.

Óscar Rodríguez Ballesteros 10/04/2023-Present Computational design of proteins.

Mikel Iraola Iñurrieta 11/04/2023-Present Topological phases in interacting-electron systems.

Fernando Peñaranda del Río 01/05/2023-Present Multiscale modelling of moiré materials.

Mihovil Bosnar 10/05/2023-06/10/2024 Condensed matter physics.

Ane Izaskun Aranburu Leiva 01/06/2023-30/09/2024 Development of luminiscent chemical sensors for the selective detection of Ba++

Galder Llorente Conde 01/06/2023-Present Organic chemistry, neuroscience.

Álvaro Pozo Larrocha 01/06/2023-Present Wave dark matter.

Shayan Edalatmanesh 05/06/2023-31/12/2024 Spin physics in graphene-based nanostructures.

Ilya Klimovskikh 19/06/2023-Present Electronic properties of quantum interfaces studied in ARPES.

Sourav Biswas 01/07/2023-Present Quantum technologies.

Haojie Guo 01/07/2023-Present Condensed matter physics and strong electron correlations in moiré quantum matter.

Yi Jiang 01/07/2023-Present HPC&IA – Magnetic properties of flat band kagome lattices studied by Inelastic neutron scattering.

Arunava Kar 01/07/2023-Present Electronic properties of flat band kagome lattices studied by ARPES.

Nico Leumer 01/07/2023-Present Spin physics in driven graphene nanostructures.

Luan Felipe Santos Martins Veríssimo 01/07/2023-30/12/2024 Computational condensed matter.

Rubén Pellicer Guridi 01/07/2023-31/12/2024 Vacancy centers in diamond for advanced quantum sensing.

Germán Eduardo Pieslinger 01/07/2023-Present Green H<sub>2</sub> generation.

Mario Zapata Herrera 06/07/2023-Present Nanophotonics.

Shivaprasad Achary Balahoju 01/09/2023-Present Organic donor-acceptor  $\pi$ -conjugated molecular systems.

Tamara Richardson 01/09/2023-Present Cosmology.

Benjamin Shirt-Ediss 14/09/2023-31/07/2024 Minimal agency and evolution.

Rodrigo Martínez Peña 01/10/2023-Present Hybrid quantum algorithms for time series analysis.

Kate Storey-Fisher 11/10/2023-25/08/2024 Cosmological structure formation.

Constance Mahony 01/11/2023-30/09/2024 Weak gravitational lensing.

Hoang Nhan Luu 20/11/2023-Present Exploring the nature of the standard cosmological model.

Moritz Frankerl 01/12/2023-Present Theory of light emission from current-driven plasmonic nanocavities.

Antoine Patt 01/12/2023-Present Theory and modelling, clathrate hydrates, porous materials.

Safa Hamreras 11/12/2023-Present Hybrid quantum algorithms for pattern recognition.

Mateo Uldemolins Nivela 01/01-31/12/2024 Theory of quantum transport in superconducting and magnetic materials.

Pablo Ezeguiel Dietz 02/01/2024-Present Neutrino physics (CEvNS) at the European Spallation Source.

Chan Young Lim 05/01/2024-Present Electronic properties of flat band kagome lattices studied by ARPES and scattering.

Ngoc Duc Le 15/01/2024-Present Nano-optics, nano-photonics and nano-plasmonics.

Juan Felipe Huan Lew Yee 15/01/2024-Present Solving the EoM for the 1RDM on quantum computing devices.

Manuel José Sánchez del Castillo 22/01/2024-Present ECC - Experimental chemistry clusterX-rays for Inorganic biochemistry lab.

Andrei Mazanik 01/04-14/09/2024 Non-equilibrium properties of unconventional Josephson junctions.

Artem Korshunov 08/04/2024-Present Uniaxial strain control of competing order parameters in complex quantum materials.

José Aarón Rodríguez Jiménez 11/04/2024-Present Quantum Lanczos methods for quantum chemistry.

Emre Bölen 15/04-31/08/2024 Diffusion of ions into polymers and calcium silicates.

Jorge Diogo Margues Laranjeira 01/05/2024-Present High-pressure computational organic chemistry. Sabine Veronika Auras 01/06-30/11/2024 Activation of COP2 on metal surfaces.

Amanda Ribeiro Guimaraes 12/06-11/12/2024 In silico design and assessment of novel polyelectrophylic chemistry agents.

Kaycee Underwood 15/06/2024-Present Novel forms of superconductivity and magnetism in two-dimensional materials.

Samuele Torelli 18/06/2024-Present Search for neutrinoless double beta decay with high pressure xenon time projection chambers.

Hanqi Pi 01/07/2024-Present Electronic structure of twisted 2 TMDs.

Nicholus Bhattacharjee 01/09/2024-Present Computational mechanistic studies of the biological function of deprotonated diradicals.

Heaiu Li 01/09/2024-Present Interactions, superconductivity, catalysis and topology in flat bands.

Tamar Meshveliani 01/09/2024-Present Massive black holes and galaxy evolution.

Christian Jenewein 02/09/2024-Present Patterns on the rocks.

Aleksander Bach Lorentzen 09/09/2024-Present Theory and simulation of time-dependent nanoelectronics.

Rafael Ramis Cortés 16/09/2024-Present Al-powered interpretation of missense variants in actionable genes.

Dulce Consuelo Guzmán Ocampo 01/10/2024-Present Molecular dynamics simulation of proteins.

Stephen Ross McMillan 01/11/2024-Present Spin qubits and graphene-based nanostructures.

Borja Aparicio Gil 18/11/2024-Present Prebiotic chemistry and origin of life.

Irene Casademont Reig 01/12/2024-Present Molecular optical properties and aromaticity.

Gonzalo Martínez Lema 06/12/2024-Present Development of the GanESS detector.

## **Research Collaborators**

Yetli Rosas Guevara 01/12/2020-30/11/2024 Theory and observation of galaxy formation.

Luis Antonio Soriano Águeda 01/02/2021-30/11/2024 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.

## PhD Students

Sara Lois Cerdeira 07/01/2020-06/01/2024 Tuning the chemical properties of graphene nanostructures.

Daniel López Cano 01/09/2020-31/08/2024 Computational cosmology

Miryam Martínez Vara 01/09/2020-31/08/2024 Search for double beta decay without neutrinos with the NEXT-100 detector.

Nischal Acharya 28/09/2020-27/09/2024 The environment of quasars & evolution of galaxies.

Nathaniel Capote Robayna 01/10/2020-30/09/2024 Polaritons in anisotropic van der Waals crystals.

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.
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.

Sara Ortega Martínez 01/01/2022-Present Cosmos: computational cosmology.

Andrei Paulau 12/01/2022-Present Theoretical chemistry.

Leire Larizgoitia Arcocha 17/01/2022-Present Development of gaseous detectors for the ESS. Tim Kokkeler 07/02/2022-06/02/2024 Transport properties of non-conventional superconducting structures.

Amitayush Jha Takur 11/04/2022-31/12/2024 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.

Julen Aduriz Arrizabalaga 13/05/2022-Present Theoretical simulation of metal-Aß complexes.

Teresa Itziar Celaya Garmendia 17/05/2022-Present Nanoneuro: optically manipulating neuronal activity with nanoparticles.

Nerea Salor Iguíñiz 01/08/2022-Present Medical physics.

Nils Hoyer 01/09/2022-29/02/2024 The cosmological evolution of Nuclear Star Clusters.

Duy Hoang Minh Nguyen 01/09/2022-Present Twisted 2D materials.

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.

Martin Irizar Landa 01/10/2022-Present Towards spin-qubits in 2.

Antonio Morales Pérez 01/10/2022-Present Artificial Intelligence algorithms for the topological control of quantum emitters.

Pablo Manuel 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.

Esteban Zingales 09/01/2023-Present Metal modulation of glucose metabolism.

Francesco Di Marcantonio 16/01/2023-15/01/2024 Simulation of quantum matter and gauge theories with tensor networks.

Mikel Elorza Romera 23/01/2023-Present Development of slow control system for the GaP detector.

Aitor González Marfil 06/03/2023-Present Deep self-supervised learning methods for bioimage analysis.

Daniel García Pina 15/03/2023-Present Magnetism in graphene nanostructures: spin chains with tunable interactions.

Paschalis Agapitos 01/04/2023-Present Complex networks methods applied to cultural analytics. Nonia Vaguero Sabater 01/04/2023-Present Quantum algorithms for quantum chemistry.

Mikel Olano Aranburu 01/06/2023-Present Moving quantum dots.

Elena Ramos Cascón 12/06/2023-Present Development, data collection and physical analysis in the WCTE and Hyper-Kamiokande experiments.

Hanae Boulehjour 01/07/2023-Present Quantum technologies – Asymmetric dilanthanide clusters as platforms for addressable gubits.

Hussen Oumer Mohammed 01/07/2023-Present Computational design of draw solutes for forward-osmosis seawater desalination

Shah Jee Rahman 01/07/2023-Present Optical trapping and levitation.

Andoni Agirre Arabolaza 01/10/2023-Present Tensor network methods for interacting electrons in quasi-1D graphene nanostructures.

Guillermo Santamaría Fernández 01/10/2023-30/09/2024 Study of phonons and charge and heat transport in molecular crystals.

Francisco Manuel Ballester Macià 16/10/2023-Present Study and application of topological phonons.

Ramón María Bergua López 16/10/2023-Present Study of fluxionality and environment effects on Pt nanoclusters for applications in catalysis.

Pablo Ramón García Valle 16/10/2023-Present Development of luminiscent chemical sensors for the selective selection of Ba++.

Carolina Adriana Iacovone 23/10/2023-Present Polymers and Soft Matter.

Marc Justin Seemann 27/10/2023-Present Experimental particle physics: towards next-generation high pressure xenon time projection chambers for neutrinoless double beta decay.

Irene Valderrama Flores 01/11/2023-Present Galaxies.

Alfonso Yubero Navarro 01/11/2023-Present Neutrino physics, surface physics.

Victor Sierka 03/11/2023-Present Design of quantum materials for channeling light and electrons.

Unai Pereira Castelo 01/12/2023-09/02/2024 Uniaxial strain tuning of the ground state of quantum materials.

Yongsong Wang 13/12/2023-Present Electronic characterization of real- and momentum-space topology of ultra flat bands.

Joan Grèbol Tomás 01/01/2024-Present Aromaticity in large conjugated circuits.

Alaitz Lecuona Isasa 01/01/2024-Present Chiral multicolor quantum dots for monitoring biologically relevant phenomena.

Alfredo Manuel Rotundo 01/01/2024-Present Photoactive anticancer drugs.

Nitin Kumar 01/02/2024-Present Catalysis and photocatalysis.

Guilherme Henrique De Oliveira 02/02/2024-Present Correlative X-ray and non-linear optical microscopy to characterise protein aggregates.

Vladyslav Chernenko 14/02-31/05/2024 Theoretical study of spin-orbit effects in scattering of electrons by surfaces. Jehyeok Ryu 29/02/2024-Present Plasmon-exciton quantum emitters for applications in quantum technologies.

Ainhoa Villoria Bárcena 01/05/2024-Present New biomolecules with Huisgenase activity: metalloproteins as biocatalysts for (3 + 2) cycloadditions.

Javier Antonio Vélez Simanca 06/05/2024-Present Chaos, magnetic materials and antiferromagnetics.

Aymeric Saunot 25/09/2024-Present Topological magnetic moiré heterostructures.

Santiago Villodre Martínez 01/10/2024-Present Condensed matter models implemented in guantum computers.

Markel García Ibarluzea 15/10/2024-Present Biophysics of potassium channels: from atomistic protein folding, to clinical testing and drug design.

Carolina Martínez Strasser 01/11/2024-Present Physics of nanostructures and advanced materials.

Alicia Omist Gálvez 16/11/2024-Present Quantum technologies.

Ludovic Donneger 01/12/2024-Present Gaseous detectors for neutrino physics.

# **Research Assistants**

Carlos Alberto Maciel Escudero 01/07/2022–31/05/2024

Ainhoa Villoria Bárcena 01/10/2022-30/04/2024

Carolina Martínez Strasser 13/10/2022–31/10/2024

Miguel Ángel Jiménez Herrera 17/10/2022–31/03/2024

Jehyeok Ryu 01/03/2023-28/02/2024

Alicia Omist Gálvez 15/07/2023–15/11/2024

Alfredo Serrano Jiménez 18/09/2023–30/09/2024

Markel García Ibarluzea 01/10/2023–14/10/2024

Irati Lizaso Berrueta 23/10/2023–Present

Martín Molezuelas Ferreras 13/11/2023–27/08/2024

Martín Gutiérrez Amigo 04/12/2023-31/08/2024

José Aarón Rodríguez Jiménez 10/12/2023–10/04/2024

Bruno Candelas Peñalba 01/01/2024–Present

David Silva Brea 01/01/2024–Present Sara Lois Cerdeira 07/01/2024–Present

Janaarthana Babu Perumal Marisami 22/01/2024–Present

Benjamin Tirado Heras 01/06–19/12/2024

Diego Herrero Carrión 14/10/2024–Present

Laura Navarro Cozcolluela 14/10/2024–Present

Shiyue Zhang 16/12/2024–Present

# Engineers

Jordi Torrent Collell 16/06/2018–Present

Eva Oblak 14/09/2020–Present

José María Benlloch Rodríguez 22/01/2022–Present

Asier Castillo Litago 02/02/2022–Present

Alejandro Taboada Fernández 11/09/2022–Present

Oier Peñasco Escandell 23/12/2024–Present

# **Technical Assistants**

Francisco López Gejo 01/01/2021–Present

Carlos Echeverría Lizarraga 01/03/2022–Present

Bruno López-Gómez Saldaña 11/09/2022-13/08/2024

José Luis López Gómez 10/02/2023–24/11/2024

Andrés Blanco Galán 03/09/2024–Present

## Internships

Aitor Echeverría Ibarbia Escuela Universitaria de Ingeniería Dual, Spain 01/09/2023-12/07/2024 Infrastructure monitoring.

Irene Plazaola Iguaran UPV/EHU, Spain 01/09/2023-01/07/2024 Chemigenetic probes based on synthetic chelators.

Gorka Acuña Pérez Zubiri Manteo, Spain 21/09/2023-18/03/2024 Administration of networked computer systems.

Alejandro Pérez Casas UPV/EHU, Spain 30/10/2023-30/01/2024 Computer engineering.

Matt Hugget Collège Sciences et Technologies - Université de Bordeaux, France 22/01-14/06/2024 Electronic structure characterization of electronic spin states in molecules.

Guillem Pey Costa Universitat de Girona, Spain 26/02-26/04/2024 Theoretical evaluation of molecular and spectroscopic properties.

Élodie Boutou Polytech Clermont-Ferrand, France 04/03-03/08/2024 Donostia natural orbital functional software.

Rebeka Rita Reszegi Universität Hamburg, Germany 18/03-30/06/2024 Chelating nanoparticles to reach metal pools in cellular environments. 01/07-01/09/2024 Nanoparticle systems for intrabacterial metal sensing.

Alejandro Martín Quevedo UPV/EHU, Spain

15/04-15/07/2024 Refinement of supercomputing use cases.

Pablo Serrano Molinero

Universidad Internacional de la Rioja (UNIR), Spain 02/05-27/06/2024 Quantum computing application to Bayesian learning.

Urko Arosa Elcoroiribe

UPV/EHU, Spain 01/06-31/07/2024 Estimation of NLOP in ionic liquids.

Idoia Cámara Garmendia UPV/EHU, Spain 01/06-31/07/2024 Theoretical design of PtGe catalyst for HOR in alkaline.

Laura Hernández Fernández Universidad de Vigo, Spain 01/06-31/07/2024 Solvent effects of biocompatible ionic liquids.

Lore Oregi Lauzirika UPV/EHU, Spain 01/06-31/07/2024 Android app development for exploring nanographenes.

Irene Plazaola Iguaran UPV/EHU, Spain 01/06-31/07/2024 Preparation of cellulose-based colorimetric sensor for heavy metal ion detection.

Cristina Sobrino Fernández Universidad Autónoma de Madrid (UAM), Spain 01/06-31/07/2024 Rhodium-catalyzed isomerization of alkenes.

Martín Zapata Ferguson Universidad Complutense de Madrid (UCM), Spain 01/06-31/07/2024 Controlling light at the nanoscale.

Iker Valle Gallegos UPV/EHU, Spain 05/06-04/08/2024 Electric circuits for the investigation of non-Hermitian lattice physics.

#### Patxi Moreno Estebánez

UPV/EHU, Spain 10/06-09/08/2024 Photoemission experiments with guantum materials.

Ane Paniagua González de Chavarri UPV/EHU, Spain 10/06-09/08/2024 Development of open-source deep learning tools for bioimage analysis.

Asier Adrián Díaz Valdivieso UPV/EHU, Spain 12/06-11/08/2024 Machine learning methods applied to the mutagenesis of ion channels.

Ander Aleson Gurruchaga UPV/EHU, Spain 19/06-18/08/2024 Aromaticity in large macrocylces.

Léa Serrano Giménez Vrije Universiteit Brussel, Belgium 26/06-26/08/2024 Rationalization of linear and non-linear optical properties.

Alejandro Blanco Peces Universidad Autónoma de Madrid (UAM), Spain 01/07-31/08/2024 Unconventional superconductivity in transition metal dichalcogenides.

Cristina Domínguez Escobar UPV/EHU, Spain 01/07-31/08/2024 Computational study of the effect of pressure on organocatalysis.

Sergio Fernández Expósito Universidad Complutense de Madrid (UCM), Spain 01/07-31/08/2024 Exploring noise impact on variational quantum eigensolvers.

Guillermo Pascua Ramón Universidad de Zaragoza, Spain 02/07-31/08/2024 Gaseous detectors for neutrino physics at the ESS. Clara Clemente Marcuello

Universidad de Zaragoza, Spain 08/07-07/09/2024 Nanophotonics in 2D materials.

Itsaso Hontoria Indart UPV/EHU, Spain 08/07-11/08/2024 Gaseous detectors for neutrino physics at the ESS.

Laura Navarro Cozcolluela Universidad de Valencia, Spain 08/07-31/08/2024 Positron-emission tomography with cryogenic crystals.

María Pérez Garrote Universidad Complutense de Madrid (UCM), Spain 08/07-31/08/2024 Gaseous detectors for neutrino physics at the ESS.

Raúl Lago Saavedra Universidad de Vigo, Spain 15/07-31/08/2024 Molecular dynamic simulations of intrinsically disordered proteins.

Alejandro Martín Rodríguez Instituto de Ciencias Fotónicas (ICFO), Spain 01/08-31/08/2024 Unconventional superconductivity in two-dimensions.

Kamil Dutkiewicz University of Warsaw, Poland 01/09-01/11/2024 Superconductivity in fractal lattices.

Carla García Gazulla Universitat de Barcelona, Spain 30/09-30/12/2024 Study on rare processes in particle physics: research on dark matter and neutrinos.

Noa Andueza Arín Zubiri Manteo, Spain 02/12/2024-Present Supercomputing Center.

# **Undergraduate Candidates**

Patxi Moreno Estebánez UPV/EHU, Spain 02/10/2023–30/06/2024 Introduction to synchrotron radiation and its use in photoemission studies.

Katy Andrea Domínguez Farinango UPV/EHU, Spain 11/10/2023–28/06/2024 Crosslinked polymers with reversible enamine-type bands.

Xabier Arrue Díaz UPV/EHU, Spain 30/09/2024–Present Experimental physics - particle physics.

Unai Miranda Redondo UPV/EHU, Spain 01/10/2024–Present Synchrotron radiation.

# Master's Degree Student

Katy Andrea Domínguez Farinango UPV/EHU, Spain 03/10/2024–Present Cyclic polymers.

# Special Assignments

Fabienne Barroso Bujans DIPC Summer Internships

Aitzol García Etxarri DIPC Transferable Skills Courses

Arantzazu García Lekue DIPC Calls for Young Researchers

Geza Giedke and Thomas Frederiksen DIPC Colloquia

David de Sancho Sánchez DIPC Seminars

Deung-Jang Choi and Nicolás Lorente Palacios DIPC Courses

Luca Salassa DIPC Workshops and DIPC Schools

Carlos Sánchez Cano PhD Seminars

Gustavo Schwartz Mestizajes program and DIPC Transdisciplinary Skills Courses

Andrés Arnau Pino, Claire Tonnelé, Francesc Monrabal Capilla and María Navarro Gastiasoro Scientific newsletter

# Gender Equality Committee

Amaia Arregi Buldain Silvia Bonoli Ricardo Díez Muiño Luz Fernández Vicente Aitzol García Etxarri Maia García Vergniory Elisa Jiménez Izal Olatz Leis Esnaola Irián Sánchez Ramírez Beatriz Suescun Rodríguez

Long visits

Pablo Herrero Gómez

Hebrew University of Jerusalem, Israel 01/10/2023-30/04/2024 Development of hardware an analysis for SABBAT project.

#### Ángel Rodríguez Alcaráz

Universidad Complutense de Madrid (UCM), Spain 02/10/2023-31/01/2024 Developing new tools for the BASQ-IBM quantum computer.

#### Chioma Ibiam Aja

Federal University of Technology Owerri, Nigeria 17/10/2023-16/09/2024 Introducing sulphons to amino acids to create super conducting capacitors.

# Visiting Researchers

## Talat Shahnaz Rahman

University of Central Florida, Orlando, FL, USA 01/12/2023-31/03/2024 01/12-31/12/2024 Theoretical and computational investigations of transport, magnetic and optical properties of functional nanomaterials.

#### Julio Alonso Martín

Universidad de Valladolid, Spain 01/12/2023-31/01/2024 01/10-30/11/2024 Interaction of small molecules with layered materials.

# Laura Barros Silva

Instituto de Química - Unicamp, Campinas, Brazil 10/12/2023-11/03/2024 Synthesis, characterization and antiviral studies of novel Pd(II) complexes with aminoadamantanes.

# Juan Faustino Aguilera Granja

Instituto de Física, Universidad Autónoma de San Luis Potosí, México 10/12/2023-09/01/2024 16/03-12/04, 04/06-31/07/2024 Nanostructures made of new components.

#### Maxim Kagan

Higher School of Economics, Moscow, Russia 15/12/2023-15/01/2024 Acoustic plasmons in novel superconducting materials.

#### Antonio Zelaquett Khoury

Instituto de Física, Universidade Federal Fluminense, Rio de Janeiro, Brazil 18/12/2023–17/03/2024 Quantum nanophotonics.

## Vladimir Nazarov

The Hebrew University of Jerusalem, Israel 01/01–31/01/2024 Optics of semiconductors and insulators beyond adiabatic local density approximation.

## Dumitru Calugaru

Princeton University, NJ, USA 11/01–30/03, 07/05–15/06/2024 SuperFlat.

# Rubén Miguel Otxoa de Zuazola

Hitachi-Cambridge Laboratory, UK 15/01–15/06/2024 Antiferromagnetism & quantum error correction.

Andrew Weber University of Missouri-Kansas City, MO, USA 01/02–30/04/2024 Thin film plasmonics.

# Joshua Renner

IGFAE - Universidade de Santiago de Compostela, Spain 01/02–31/05/2024 HyperK / WCTE radioactive source development.

# Joseph Richard Manson

Clemson University, SC, USA 01/02–28/03, 01/09–31/10/2024 Electron-phonon interactions at surfaces.

# Tyann Dumerchat

Centre de Physique des Particules de Marseille, Aix-Marseille Université, France 12/02–15/03/2024 Cosmology with peculiar velocity clustering.

# Sergi Danés Pibernat

Universitat de Girona, Spain 15/02–15/05/2024 Theoretical evaluation of molecular and spectroscopic properties.

#### Zenan Dai

Shanghai Jiao Tong University, China 15/02–15/09/2024 Topological insulators.

# Pau Besalú Sala

Institut de Química Computacional i Catàlisi, Facultat de Ciències, Girona, Spain 26/02–08/04/2024 Theoretical evaluation of molecular and spectroscopic properties.

# Andrey Borissov

Institut des Sciences Moléculaires d'Orsay - CNRS - Université Paris-Saclay, France 01/03–30/04, 15/10–15/12/2024 Quantum plasmonics, strong field emission, electron transport in plasmonic gaps.

# Simon White

Max Planck Institute for Astrophysics, Garching bei München, Germany 03/03–30/03/2024 Cosmological structure formation.

# Matteo Santini

Università di Bologna, Italy 11/03–09/07/2024 Angular redshift fluctuations in extragalactic mappings.

# João Pedro Vieira de Mendonça Santos

Faculty of Physics, University of Warsaw, Poland 20/03–22/06/2024 Non Fermi liquid behavior in Hubbard ladders.

# Heba Kandil

National Research Center, Dokki, Egypt 21/03–14/09/2024 Exploring polysaccharide materials: innovating wound healing patches for optimal recovery.

#### Seok Gyeong Yoon The University of Chicago, IL, USA 29/03–29/08/2024

29/03–29/08/2024 ERC-ESSCEvNS.

# Petru Milev

Wrocław University of Science and Technology, Poland 30/03–28/06/2024 Efficient methodologies for computing response propreties of molecules and materials.

# José Ángel Hernando Morata

Instituto Galego de Física de Altas Enerxías (IGFAE) - Universidade de Santiago de Compostela (USC), Spain 01/04–30/06/2024 Neutrinos.

# Gernot Frenking

Philipps-Universität Marburg, Germany 01/04–30/05/2024 Quantum chemical analysis of the chemical bond.

# Oleg Dolgov

Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia 01/04–30/06/2024 Electronic excitations and superconducting instability in solids.

# Agustín Rodríguez Medrano

Instituto de Astronomía Teórica y Experimental (IATE - Conicet), Córdoba, Argentina 01/05–30/07/2024 BACCO simulations.

# Bárbara Andrade dos Santos

ICFO – The Institute of Photonic Sciences, Castelldefels, Spain 01/05/2024–01/05/2025 Real-time evolution of lattice gauge theories using modern quantum devices.

# Paula Natalia Abufager

Instituto de Física Rosario, Argentina 01/05–01/07/2024 Electronic, magnetic and transport properties at the nanoscale.

# Eric Switzer

University of Central Florida, Orlando, FL, USA 05/05–28/06/2024 Developing new tools for the BASQ-IBM quantum computer.

# Karol Angélica Chim Ramirez

Institute of Radio Astronomy and Astrophysics (IRyA), UNAM, Morelia, México 06/05–01/07/2024 Parametric and environmental study of the formation and evolution of stellar bars in a cosmological context.

## Peter Saalfrank

University of Potsdam, Germany 11/05–22/06/2024 Hot-electron mediated chemistry at metal nanoparticles.

## In-Sang Yang

Ewha Womans University, Seoul, South Korea 13/05-13/08/2024Spin rotational excitations in hexagonal *R*MnO<sub>3</sub> (R=Y, rare-earths).

## Oleg Prezhdo

University of Southern California, Los Angeles, CA, USA 25/05–25/08/2024 Excited state dynamics in novel nanoscale materials for optoelectronic applications.

## Stephanie Louise Yardley

Northumbria University, Newcastle, UK 01/06–01/09/2024 Solar Physics/ Space weather.

## Christian Jenewein

Instituto Andaluz de Ciencias de la Tierra (IACT), Armilla, Granada, Spain 01/06–31/08/2024 Patterns on the rocks.

## Godfrey Gumbs

Hunter College, City University of New York, USA 01/06–30/06/2024 Thermoelectric response of magic-angle twisted bilayer graphene in external fields.

# Elton Gomes Dos Santos

James Clerk Maxwell Building, The University of Edinburgh, UK 01/06–01/09/2024 Correlated properties based quantum technologies.

#### Francisco José García Vidal

Facultad de Ciencias, Universidad Autónoma de Madrid (UAM), Spain 01/06–31/07/2024 Quantum light-matter interaction.

#### Juan Pablo Echeverry Enciso

Universidad de Ibagué, Colombia 01/06–30/07/2024 Electron-plasmon coupling in TiSe<sub>2</sub> monolayers and bilayers.

#### Blanca del Rosal Rabes

RMIT University, Melbourne, Australia 01/06–30/06/2024 Nanoneuro.

## Edgar Martín Salazar Canizales

University of Arizona, Tucson, AZ, USA 03/06–28/06/2024 Large scale structure modeling.

## Eduardo Rozo

University of Arizona, Tucson, AZ, USA 03/06–28/06/2024 Modeling of large scale structure.

## Mads Brandbyge

Technical University of Denmark (DTU), Kongens Lyngby, Denmark 03/06–07/07/2024 Electron transport in carbon nanostructures.

## Dmitri Efremov

Institute for Solid State Physics and Material Research (IFW), Dresden, Germany 07/06–06/07/2024 Charge excitations in superconducting materials.

## Haozhe Tong

Nanyang Technological University (NTU), Singapore 09/06–09/08/2024 Hyperbolic nanooptics.

## Pavel Jelinek

Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic 17/06–17/07/2024 Magnetism at surfaces.

#### Rafael Yuste Rojas

Columbia University, New York, NY, USA 01/07–20/08/2024 Neurophysics.

#### Andrey Vasenko

HSE University, Moscow, Russia 01/07–30/09/2024 Photo-excitation dynamics in nanoscale systems.

# Alejandro Martín Rodríguez

ICFO, Castelldefels, Spain 01/07–31/07/2024 STM/STS measurements on 2D materials.

## Luis Martín Moreno Instituto de Nanociencia y Materiales de Aragón, Zaragoza, Spain 01/07–31/07/2024 Theory on nanophotonics.

## Nikolay Kabachnik

European XFEEL GmbH, Schenefeld, Germany 01/07–30/09/2024 Theoretical description of time-delay in photoemission from solid surfaces.

## María Ángeles Hernández Vozmediano

Instituto de Ciencia de Materiales de Madrid, Spain 01/07–31/07/2024 Topological semimetals. Semimetal topologikoak.

# Gabriel Alejandro Cwilich

Yeshiva University, New York, NY, USA 01/07–31/12/2024 Modeling of networks applied to vehicular traffic and similar problems.

# Ivano Sarra

Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, Italy 02/07–29/08/2024 Detectors for neutrino physics.

## Sergio Ceravolo

Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, Italy 02/07–29/08/2024 Detectors for neutrino physics.

## Rodrigo Humberto Aguilera del Toro

Universidad de Valladolid, Facultad de Ciencias, Spain 04/07–01/08/2024 12/12/2024–12/01/2025 On the quest of new magnetic 2D materials.

## Felix von Oppen

Dahlem Center for Complex Quantum Systems and Freie Universität Berlin, Germany 06/07–04/08/2024 Theory of the quantum twisting microscope.

#### Leonid Glazman

Yale University, New Haven, CT, USA 13/07–11/08/2024 Phonon spectroscopy with the quantum twisting microscope.

# Alejandro González Tudela

Instituto de Física Fundamental, Madrid, Spain 14/07–15/08/2024 Topological quantum optics.

# Yuval Oreg

Weizmann Institute of Science, Rehovot, Israel 19/07–05/08/2024 Novel properties of van der Waals layered systems.

#### Victor Oluwapemi Adebayo Paul Sabatier University, Toulouse, France 29/07–22/09/2024

29/07–22/09/2024 Mechanism of doublet-triplet energy transfer for photon upconversion.

## Mohammad Monir

KU Leuven, Belgium 01/08–01/10/2024 Magnetic anisotropy in organic polyradicals.

# Igor Karnaukhov

GV Kurdyumov Institute for Metal Physics of the NAS of Ukraine, Kyiv, Ukraine 01/08–30/10/2024 Topological insulators and superconductors.

# Tairzhan Karabassov

HSE University, Moscow, Russia 01/08–31/08/2024 Superconductivity in topologically nontrivial materials.

# Sergio Carbajo García

UCLA, Los Angeles, CA, USA 01/08–31/08/2024 Topological nanophotonics.

# Guillermo Pedro Acuña

University of Fribourg, Faculty of Science and Medicine, Switzerland 01/08–31/10/2024 Chiral light matter interactions at the nanoscale.

# Pablo Ares García

Facultad de Ciencias, Universidad Autónoma de Madrid (UAM), Spain 15/08–15/09/2024 AFM polarization in moiré materials.

# Ziya Aliyev

Baku State University, Azerbaijan 25/08–25/09/2024 Materials physics of magnetic topological insulators.

# Alexander Yaresko

Max Planck Institute for Solid State Research, Stuttgart, Germany 01/09–30/09/2024 Spin-polarized photoemission from the surface of antiferromagnet.

# Leonid Sandratskii

Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic 01/09–30/11/2024 Magnons in altermagnets: symmetry aspects and first-principles calculations.

# Ceferino López Fernández

ICMM (CSIC), Madrid, Spain 01/09–30/09/2024 Disorder photonics. Stephen Ross McMillan Universität Konstanz, Germany 12/09–31/10/2024 Spin dynamics in nanographenes.

Kurt Walsen Bluee-Blatter Universidad Diego Portales (UDP), Santiago, Chile 16/09–07/12/2024 Cosmological simulations.

Giorgio Benedek Università di Milano-Bicocca, Italy 16/09–23/10/2024 Surface dynamics and electron phonon interaction.

#### Valeria Aylen Cristiani

Instituto de Astronomía Teórica y Experimental (IATE), Córdoba, Argentina 19/09–17/12/2024 Properties of disks and spheroids in galaxies belonging to hydrodynamic simulations.

#### Nischal Acharya

DIPC, Donostia/San Sebastián, Spain 28/09/2024–28/09/2025 Connecting active galactic nuclei to host galaxy properties.

#### Julio Navarro

University of Victoria, Canada 01/10/2024–31/03/2025 Dark matter clues from the faintest galaxies in the universe.

#### Anabel Lam Barandela

Universidad de La Habana, Cuba 01/10-31/10/2024 Cyclic polymers.

Nathaniel Capote Robayna DIPC, Donostia/San Sebastián, Spain 01/10–30/10/2024 Polaritons in anisotropic van der Waals crystals.

Matyas Nachtigall University of Luxembourg, Luxembourg 07/10–31/12/2024 Quantum treatments of nanophotonic systems.

#### Roberto José Javier Assef Trebilcock

Facultad de Ingeniería y Ciencias, Universidad Diego Portales (UDP), Santiago, Chile 15/10–15/11/2024 GN and galaxy evolution.

#### Luis Alberto Montero Cabrera

Universidad de La Habana, Facultad de Química, Cuba 01/11–30/11/2024 Photophysics of molecular photovoltaic devices.

#### Amaia Elizaran Mendarte

UPV/EHU, Leioa, Spain 15/11/2024–28/02/2025 Neural networks optimisation in data scarcity scenarios.

#### Junze Deng

Aalto University, Espoo, Finland 30/11/2024–30/06/2025 Study on kagome flat band materials.

#### Haoyu Hu

Princeton University, NJ, USA 01/12/2024–01/10/2025 SuperFlat.

#### An Wei

University of Science and Technology Beijing, China 11/12/2024–10/12/2025 Quantum treatments of molecule-nanoresonator coupling.

#### Maxim Kagan

Higher School of Economics, Moscow, Russia 16/12/2024–14/01/2025 Investigation of doping dependence and plasmon poles of the dielectric function of cuprate high-T-c superconductors.

# Short Visits

#### Rene Christian Urbina Jimenez

SPEC (CNRS-CEA) Université Paris-Saclay, Gif-sur-Yvette, France 08/01–11/01/2024 The exciting life of quasiparticles trapped between superconductors.

#### Marcelo Goffman

SPEC (CNRS-CEA) Université Paris-Saclay, Gif-sur-Yvette, France 08/01–11/01/2024 The exciting life of quasiparticles trapped between superconductors.

#### Anya Paopiamsap

University of Oxford, UK 09/01–13/01/2024 Large scale structure of the universe.

#### David Izquierdo Villalba

Università degli Studi di Milano-Bicocca, Italy 14/01–26/01/2024 Black hole growth and spin evolution.

#### Carolina Cuesta Lázaro

MIT, Cambridge, MA, USA 15/01–18/01/2024 Cosmological constraints from galaxy surveys.

#### Diego Herrero Carrión

Universidad Complutense de Madrid (UCM), Spain 21/01–25/01/2024 L-Galaxies.

#### Mohammadreza Ayromlou Heidelberg University, Germany 21/01–26/01/2024 L-Galaxies.

## Fabian Schmidt

Max Planck Institute for Astrophysics, Garching, Germany 28/01–02/02/2024 Forward models for large-scale structure.

## Wei Xiong

University of California, San Diego, CA, USA 29/01–02/02/2024 Energy redistribution among vibrational degrees of freedom in molecular layers.

## Jorge Iván Cárdenas Gamboa

Max Planck Institute for Chemical Physics of Solids, Dresden, Germany 03/02–24/02/2024 Non-collinear magnetism / Phonon calculation.

## Christian Jenewein

Instituto Andaluz de Ciencias de la Tierra (IACT), Armilla, Granada, Spain 04/02–07/02/2024 Mineral self-organization and origin of life.

## Jorge Olmos Trigo

Facultad de Ciencias, Universidad de La Laguna, Spain 06/02–18/02/2024 Optical torgues at the nano-and-microscale.

## Samuele Torelli

Gran Sasso Science Institute, L'Aquila, Italy 07/02–10/02/2024 Search for neutrinoless double beta decay with high pressure xenon time projection chambers.

## Arzhang Ardavan

The Clarendon Laboratory, University of Oxford, UK 15/02–15/02/2024 Experimental implementation of quantum error detection using hyperfine-coupled nuclear qudits.

## Tim Kokkeler

University of Twente, Enschede, Netherlands 18/02–25/02, 12/10–22/10/2024 Nonlinear sigma model for materials with magnetic sublattices.

## Alexander Golubov University of Twente, Enschede, Netherlands 21/02–25/02/2024 Superconductor, topological insulator hybrid structures.

## Fabio Donati Center for Quantum Nanoscience, Ewha Womans University, Seoul, South Korea 21/02–24/02/2024 Lanthanide atoms on superconducting surfaces.

#### Magdalena Marganska-Lyzniak

Institute for Theoretical Physics, University of Regensburg, Germany 02/03–10/03/2024 Gipuzkoa Quantum.

#### Norhan Omar

Institut des Sciences Moléculaires, Talence, France 03/03–08/03/2024 DALTON - how hydrogen desorption and adsorption are influenced on tungsten by oxygen and nitrogen?

## Guinevere Kauffmann

Max Planck Institute for Astrophysics, Garching, Germany 04/03–31/03/2024 Physical properties of galaxies in DESI bright galaxy survey; stellar halos of low mass galaxies.

## Iván Fernandez-Corbatón

Karlsruhe Institute of Technology, Germany 07/03–08/03/2024 Light-matter interactions.

## Rein Ulijn

Advanced Science Research Center CUNY, NY, USA 10/03–11/03/2024 Materials discovery through exploration of biomolecular space.

## Martin Tomterud

University of Bergen, Norway 11/03–15/03/2024 Temperature dependent properties of two dimensional materials.

#### Roberto Cammi

Università di Parma, Italy 12/03–14/03/2024 Effect of pressure on tunneling in organic reactions.

## Mu-Kun Li

Waseda University, Tokyo, Japan 16/03–27/03/2024 Evindence of time-dilation in topologically protected antiferromagnetic textures.

# Mikhail Otrokov

Instituto de Nanociencia y Materiales de Aragón, Zaragoza, Spain 18/03–21/03, 13/05–16/05, 16/12–20/12/2024 Magnetic topological insulators.

# Philippe Roncin

Université Paris-Saclay, Orsay, France 25/03–04/04/2024 Inelastic diffraction of atoms on surfaces.

# Julia Contreras García

Sorbonne Université, Paris, France 04/04–04/05, 11/12–20/12/2024 Non covalent interactions and electron delocalization.

# Antonio Hernando Grande

Universidad Complutens, Madrid, Spain 08/04–12/04/2024 Magnetism in neurons.

# Fernando Aguilar-Galindo Rodríguez

Universidad Autónoma de Madrid (UAM), Spain 08/04–12/04/2024 Electron dynamics under the effect of strong laser pulses.

# Jacopo Dosso

Università degli Studi di Trieste, Italy 10/04–12/04/2024 Reinventing dihydrophenazine systems: from smart materials to catalysis.

#### Ewa Lokas

Nicolaus Copernicus Astronomical Center (CAMK PAN), Warsaw, Poland 11/04–13/04/2024 Tidally induced bars in galaxies.

#### Thales Gutcke

Institute for Astronomy University of Hawaii, Hilo, HI, USA 14/04–20/04/2024 Dwarf galaxy simulations.

## Guillem Aromi Bedmar

Universitat de Barcelona, Spain 17/04–18/04/2024 Spin qubit molecules.

## Mahammad Babanli

Institute of Catalysis and Inorganic Chemistry named after Academician M. Nagiyev, Baku, Azerbaijan 21/04–27/04/2024 Development of new magnetic topological insulators.

## Cyril Aymonier

Institute for Condensed Matter Chemistry of Bordeaux (ICMCB), Pessac, France 22/04–26/04/2024 LTC green concrete.

## Jacek Styszynski

Institute of Physics, University of Szczecin, Poland 26/04–04/05/2024 Relativistic effects in chemical bonding analysis.

## Beñat Martínez de Aguirre Jokisch

Technical University of Denmark (DTU), Lyngby, Denmark 28/04–05/05/2024 Nano-optics, nano-photonics and nano-plasmonics.

# José Manuel Caridad Hernández

Universidad de Salamanca, Spain 28/04–30/04/2024 Graphene-based heterostructures for Terahetz detection technology.

## Kasper Moth-Poulsen

Universitat Politècnica de Catalunya (UPC), Barcelona, Spain 29/04–30/04/2024 Synthetic chemistry for energy storage, solar energy, sensors and molecular electronics.

# Zhiyu Hu

Zhangjiang Institute for Advanced Study, Shanghai Jiao Tong University, China 29/04–30/04/2024 Nano-fire technology and nanocatalysts.

## Anastasia Vyalikh

Technical University Dresden, Germany 01/05–04/05/2024 Low dimensional functional materials.

# Eloy Ramos Córdoba

Instituto de Química Avanzada de Cataluña - CSIC, Barcelona, Spain 10/05–19/05/2024 Development of new density functional approximations.

## Karolina Slowik

Nicolaus Copernicus University in Toruń, Poland 15/05–29/05/2024 Optical properties of grahene nanostructures.

## Marta Pelc

Nicolaus Copernicus University in Toruń, Poland 15/05–29/05/2024 Investigating electro-optical properties of graphene nanoflakes with adatoms.

## Anna Seiler

ETH Zürich, Switzerland 20/05–25/05/2024 Optics, electronics and magnetism in 2D materials.

#### Giovanni Aricò

University of Zurich, Switzerland 20/05–31/05/2024 Cosmological implications of dark energy.

#### Garnett Bryant

National Institute of Standards and Technology, Gaithersburg, MD, USA 27/05–31/05/2024 Quantum plasmonics.

María del Valle Palomo Ruíz IMDEA Nanociencia, Madrid, Spain 31/05–31/05/2024

Quantum dots and peptide-based sensors to develop and improve drug selection in neurodegenerative diseases.

#### Gorm Ole Steffensen

Instituto de Ciencia de Materiales de Madrid (ICMM), Spain 06/06–08/06/2024 Non equilibrium transport in proximitized InAs-Al nanowires.

Rodney Dewayne Priestley Princeton University, NJ, USA 10/06–13/06/2024 Glass transition in polymers.

Zoltán Haiman Pupin Laboratories, Columbia University, New York, NY, USA 10/06–16/06/2024 Massive black holes.

Latha Venkataraman Columbia University, New York, NY, USA 13/06–16/06/2024 Electroluminescence at the nanoscale.

Sebastian Kozuch Ben-Gurion University of the Negev, Be'er Sheva, Israel 21/06–27/06/2024 Tunneling in organic reaction under pressure.

Simon Mun Gwangju Institute of Science and Technology, South Korea 25/06–27/06/2024 Surface science with ambient pressure XPS.

#### Joaquín González Nuevo Gónzalez

Universidad de Oviedo, ICTEA, Oviedo, Spain 27/06–27/06/2024 Cosmology with magnification bias.

Adrian Feiguin Northeastern University, Boston, MA, USA 30/06–03/07/2024 Software ecosystem.

Juan Pablo Ortega School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 01/07–06/07/2024 Quantum reservoir systems for machine learning.

# Lyudmila Grigoryeva Faculty of Mathematics and Statistics University of St. Gallen, Switzerland

01/07–06/07/2024 Quantum reservoir systems for machine learning.

## Michael Edward Flatté

University of Iowa, IA, USA 03/07–07/07/2024 Spintonics and superconductors.

Adiel Stern

Weizmann Institute of Science, Rehovot, Israel 07/07–27/07/2024 Flat bands in multi-layer systems.

Stephan Roche Catalan Institute of Nanoscience and Nanotechnology (ICN2), Bellaterra, Spain 08/07–19/07/2024 Spintronics, quantum technologies and advanced electronics.

Charles Marcus University of Washington, Seattle, WA, USA 10/07–17/07/2024 Experimental research on quantum materials.

Javier García de Abajo ICFO - Institut de Ciències Fotòniques, Castelldefels, Spain 13/07–19/07, 21/09–27/09/2024 Plasmonics in atomically thin crystalline silver films.

#### Chen Fang

Institute of Physics, Chinese Academy of Sciences, Beijing, China 13/07–20/07/2024 Many-body scar dynamics and open quantum systems.

#### Elia Strambini

Istituto Nanoscienze (CNR-NANO), Pisa, Italy 15/07–27/07/2024 Magnetic Josephson junctions and superconducting diodes.

#### Javier Aguilar Sánchez

Università degli Studi di Padova, Padua, Italy 15/07–18/07/2024 Binomial quantum trajectories.

Mitchell Luskin

University of Minnesota, Minneapolis, MN, USA 21/07–31/07/2024 Two-dimensional materials.

#### Lisa Randall

Harvard University, Cambridge, MA, USA 22/07–26/07/2024 Warped five-dimensional geometry in particle physics, cosmology, and more formal theory.

#### Alfredo Levy Yeyati

Universidad Autónoma de Madrid (UAM), Spain 22/07–29/07/2024 Towards a new Shiba Qubit based on superconductor-semiconductor hybrid quantum dots.

Zhipeng Wang Tohoku University, Sendai, Japan

23/07–25/07/2024 Magnetic molecules on superconductors.

Daniel Cooke

University of Texas at Austin, TX, USA 27/07–30/07/2024 Nanoneuro.

## Christoph Strunk

University of Regensburg, Germany 28/07–31/07/2024 Superconducting diode effect.

# Yao Zhang

University of Science and Technology of China, Hefei, Anhui, China 03/08–07/08/2024 Atomistic description of surface enhanced raman spectroscopy.

# José Francisco Toledo Alarcón

Universitat Politècnica de València, Gandia, Spain 19/08–21/08/2024 Experimental particle physics.

# Joaquín Armijo

Kavli Institute for the Physics and Mathematics of the Universe (IPMU), Kashiwa, Japan 19/08–23/08/2024 Modelling of the large-scale structure of the universe.

## Matteo Zennaro

University of Oxford, UK 28/08–06/09/2024 Cosmological structure formation.

## Raúl Lago Saavedra

Universidad de Vigo, Spain 01/09–15/09/2024 Molecular dynamic simulations of intrinsically disordered proteins.

Julio Gómez Herrero Universidad Autónoma de Madrid (UAM), Spain 03/09–05/09/2024 Proximity microscopy: the eyes of nanotechnology.

## Thomas Eckl

Robert Bosch, Renningen, Germany 17/09–19/09/2024 Achieving quantum utility for industrial applications in materials simulation. Claudio Savarese The University of Manchester, UK 18/09-20/09/2024 Development of dark matter detectors.

Marco Montalti Università di Bologna, Italy 23/09-28/09/2024 Mineral self-organisation.

Michele Parrinello Fondazione Istituto Italiano di Tecnologia, Genoa, Italy 25/09-27/09/2024 Do we really understand catalysis?

#### José Luís Lado Villanueva

Aalto University, Espoo, Finland 29/09-01/10/2024 Hamiltonian learning, triplons, and high-order topological order in engineered nanoscale quantum magnets.

#### Lexin Ding

Ludwig-Maximilians-Universität München, Germany 29/09-05/10/2024 Quantum information theory for studying chemical bonding.

#### Nelson David Padilla

Instituto de Astronomía Teórica y Experimental (IATE), Córdoba, Argentina 30/09-04/10/2024 Warm dark matter simulations.

#### Manfred Mark

Universität Innsbruck, Institut für Experimentalphysik, Austria 01/10-05/10/2024 Novel quantum phases in ultracold dipolar gases.

#### Steen Rasmussen

University of Southern Denmark, Odense, Denmark 05/10-25/10/2024 Physics of living materials.

#### Salvador Miret Artés

Instituto de Física Fundamental, Madrid, Spain 07/10-11/10/2024 Fundamentals of guantum mechanics and stochastic processes.

#### Jens Oliver Stücker

University of Vienna, Austria 13/10-20/10/2024 Warm dark matter simulations.

Rik Broekhoven

Delft University of Technology, The Netherlands 13/10-16/10/2024 Efficient algorithm for dispersion of Yu-Shiba-Rusinov chains on a superconducting surface.

#### Martin Tomterud

University of Bergen, Norway 20/10-24/10/2024 Temperature dependent properties of two dimensional materials.

#### Azadeh Moradinezhad

Laboratoire d'Annecy de Physique Théorique (LAPTh), Annecy, France 20/10-23/10/2024 Primordial non-gaussianity in the universe.

#### Marcin Bartosz Semczuk

Institut de Ciències del Cosmos (ICCUB). Universitat de Barcelona, Spain 24/10-25/10/2024 Theory and observation of galaxy formation.

#### Sara Capponi

IBM Almaden Research Center, San Jose, CA, USA 26/10-03/11/2024 Nanoneuro.

#### Shalitha Shrimantha Bandara Pathiranage

Queen Mary University of London, UK 03/11-15/11/2024 Near-field microscopy with epitaxially-grown h-BN.

#### Yang Hao

Queen Mary University of London, UK 07/11-09/11/2024 Near-field microscopy with epitaxially-grown h-BN.

#### Valentina De Romeri

Instituto de Física Corpuscular (IFIC), Paterna, Spain 11/11-15/11/2024 Coherent elastic neutrino-nucleus scattering in the standard model and beyond.

#### James De Yoreo

Pacific Northwest National Laboratory, Richland, WA, USA 20/11-23/11/2024 In situ studies of hierarchical nucleation pathways in silicate and carbonate systems.

#### Chunli Huang

University of Kentucky, Lexington, KY, USA 03/12-05/12/2024 Superconductivity and spin-transport in two dimensional materials

#### Juan Faustino Aquilera Granja

Universidad Autónoma de San Luis Potosí, México 06/12-18/12/2024 Nanostructures made of new components.

#### Abhishek Ghosh

Nicolaus Copernicus University in Toruń, Poland 08/12-22/12/2024 Graphene mediated adatom interaction.

#### Abel Rojo Francàs

Universitat de Barcelona, Spain 09/12-13/12/2024 Few guantum particles on a fractal lattice.

#### Diego Martín Cano IFIMAC, Universidad Autónoma de Madrid (UAM), Spain 09/12-11/12/2024

Theory of interactions between light and molecules in nanoenvironments.

## Yann Fichou

CBMN/CNRS, Pessac, France 12/12-13/12/2024

Understanding the modulators of tau amyloid aggregation pathways.

## Aurelia Chenu

University of Luxembourg, Luxembourg 18/12-21/12/2024 Control of open quantum systems.

# Administration and Services



# General Management

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Olatz Leis Esnaola Head of Finance & Accounting and R+D+i Project Management

Txomin Romero Asturiano Head of Supercomputing Center

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

# Administration

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María del Mar Álvarez San Martín Human Resources and Administration

Xabier De la Torre Arostegui Public Procurements and Administration As of 25/11/2024

Amaia Etxaburu Munduate President's Assistant

Nerea Fariñas Conde Public Procurements and Administration End of contract: 05/05/2024

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Natasha Nedashkivska Finance & Accounting and Administration

**Yannick Sáenz Augusto** Finance & Accounting and Administration

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Ekain Ugalde Goldarazena

Jarvin Baca Sánchez As of 04/11/2024

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Marina Santos Ovejero Jone Zabaleta Llorens

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Aitor Echeverría Ibarbia HPC Infrastructure Maintenance

Luz Fernández Vicente Help Desk & Microinformatics

Daniel Franco Barranco HPC Resources Administration End of contract: 31/10/2024

Belén Isla Rodríguez HPC Services Design

Diego Lasa Goicuria HPC Software & Applications End of contract: 12/03/2024

Carmen Martín Pulpón Security, Web & Networks

Iker Ortiz de Luzuriaga HPC Resources Administration

Carlos Pérez Miguel HPC Software and Applications As of 11/06/2024

Youssef Raoudi Zakir Help Desk & Microinformatics

Unai Sainz de la Maza Gamboa Computing System Management

Julen Suárez Ventosa HPC Resources Administration End of contract: 26/11/2024

1 The exciting life of quasiparticles trapped between superconductors 10/01/2024 Cristian Urbina SPEC (CNRS-CEA) Université Paris-Saclay, Gif-sur-Yvette, France

2 The mathematics of the periodic table of the elements 26/01/2024 Jan Philip Solovej University of Copenhagen, Denmark

3 Ultrafast dynamics of molecular polaritons 31/01/2024 Wei Xiong University of California, San Diego, CA, USA

08/02/2024 Johannes Gierschner IMDEA Nanociencia, Madrid, Spain

09/02/2024 Samuele Torelli Gran Sasso Science Institute, L'Aquila, Italy

for TeraHz emission 13/02/2024 Albert Fert Université Paris-Saclay, Orsay, France

# Seminars

4 Scientific misconduct in current materials research: aspects, conditions and perspectives

5 Feasibility of a directional solar neutrino measurement with the CYGNO/INITIUM experiment

6 Orbitronics: orbital currents induced by currents in interfacial orbital textures or by light

7 Experimental implementation of quantum error detection using hyperfine-coupled

nuclear gudits 15/02/2024 Arzhang Ardavan

The Clarendon Laboratory, University of Oxford, UK

8 Structured quantum optics (part 1) 21/02/2024 Antonio Zelaquett Khoury

Universidade Federal Fluminense, Rio de Janeiro, Brazil

9 Addressing sub-meV interactions and multi-orbital configurations with X-ray absorption spectroscopy 23/02/2024 Fabio Donati

Institute for Basic Science (IBS), Ewha Womans University, Seoul, South Korea

# 10 Structured quantum optics (part 2)

28/02/2024 Antonio Zelaquett Khoury Universidade Federal Fluminense, Rio de Janeiro, Brazil

# 11 Algebraic tools for light-matter interaction

07/03/2024 Ivan Fernandez-Corbaton Karlsruhe Institute of Technology, Germany

12 Electronic interactions and superconductivity with fragmented Fermi surface 08/03/2024 Magdalena Marganska Institute for Theoretical Physics, University of Regensburg, Germany

# 13 Materials discovery through exploration of biomolecular space 11/03/2024

Rein Ulijn Advanced Science Research Center CUNY, NY, USA

14 Spins in mesoscopic and topological systems for quantum computing and spintronics 21/03/2024 Vitaly Golovach CFM UPV/EHU-CSIC and DIPC, Donostia/San Sebastián, Spain

15 Diversity Matters - some strategies that could broaden participation 22/03/2024 Talat S Rahman University of Central Florida, Orlando, FL, USA

16 Reinventing dihydrophenazine systems: from smart materials to catalysis 12/04/2024 Jacopo Dosso Università degli Studi di Trieste, Italy

17 Constructing new models to predict superconductivity 15/04/2024 Julia Contreras García CNRS-Sorbonne Université, France

18 Heterometallic lanthanide coordination complexes for guantum technologies 17/04/2024 Guillem Aromí Universitat de Barcelona, Spain

19 Open science with Springer Nature (policies and tools) 18/04/2024 Asja Prohic Head of Academic Affairs, Springer Nature, France

20 Utility-scale quantum computing in your own quantum computational workflows 23/04/2024 Pedro Rivero IBM Quantum, NY, USA

21 Temporal aspects of electron scattering: superluminality, negative transit time, and attosecond chronoscopy 25/04/2024 Eugene Krasovskii UPV-EHU, DIPC and IKERBASQUE, Donostia/San Sebastián, Spain

22 From nanofire to micro-TEG chip power generation technology 30/04/2024 Zhiyu Hu Shanghai Jiao Tong University, China

23 Graphene-based heterostructures for Terahetz detection technology 30/04/2024 José Caridad University of Salamanca, Spain

24 Exploring the role of nuclear magnetic resonance (NMR) spectroscopy in the study of biorelevant nanocomposites and electrochemical reactions 03/05/2024 Anastasia Vyalikh Technical University Dresden, Germany

25 From data analysis to machine learning, the mathematical connection that makes scientists so valuable in tech companies 10/05/2024 Roberto Sanchís Ojeda Spotify, Spain

26 Quantum interference effects in molecular nanoelectronics: theory and applications 13/05/2024 Angelo Valli Budapest University of Technology and Economics, Hungary

27 A personal perspective on simulations of biomolecules: challenges and opportunities 23/05/2024 Xabier López UPV/EHU and DIPC, Donostia/San Sebastián, Spain

28 Magnetic molecules: structure, spectroscopy, and dynamics

24/05/2024 Jon Kragskow Univerty of Bath, UK

29 Topological properties of altermagnets 27/05/2024 Rafael Fernandes

University of Minnesota, Minneapolis, MN, USA

Ewha Womans University, Seoul, South Korea

30 Hybrid halide perovskites: Taking advantage of ion migration and stability 27/05/2024 Pablo Docampo University of Glasgow, UK

31 Resonance Raman study of spin rotational excitations in hexagonal RMnO<sub>3</sub> (R = rare earths, Y) 29/05/2024 In-Sang Yang

32 Neutron beams for irradiation applications at the Rutherford Appleton Laboratory 30/05/2024 Carlo Cazzaniga UKRI-STFC, UK

33 Quantum dots and peptide-based sensors to develop and improve drug selection in neurodegenerative diseases 31/05/2024 Valle Palomo IMDEA Nanociencia, Madrid, Spain

34 Quantum computing cosmology. Computing the universe 06/06/2024 George F. Smoot Hong Kong University of Science and Technology, DIPC, Hong Kong and Spain

35 The formation and growth of massive black holes 12/06/2024 Zoltan Haiman Columbia University, New York, NY, USA

36 Photochemistry without light: molecules in cavities 12/06/2024 Peter Saalfrank Department of Chemistry, University of Potsdam, Germany

37 Conductance and electroluminescence in single-molecule devices 14/06/2024 Latha Venkataraman Columbia University, New York, NY, USA

38 Development of quantum algorithms for electronic structure calculations 17/06/2024 Matthieu Saubanere LOMA, Bordeaux, France

39 Heavy atom tunneling: when molecules disobey the reactivity textbook 24/06/2024 Sebastian Kozuch Ben-Gurion University of the Negev, Be'er Sheva, Israel

26/06/2024 Bongjin Simon Mun Gwangju Institute of Science and Technology, South Korea

41 From femtoseconds to nanometers: an overview of ultrafast laser spectroscopy and atomic force microscopy at boise state university 27/06/2024 Paul Davis Boise State University, Boise, ID, USA

42 Time dependent approach to non-equilibrium spectroscopies 01/07/2024 Adrian Feiguin Northeastern University, Boston, MA, USA

- 40 A study of surface oxides on Pt<sub>3</sub>Ni(111) and Pt<sub>3</sub>Co(111) using ambient pressure STM and XPS

43 Quantum metrology in the ultra-strong coupling limit 08/07/2024 Karol Gietka University of Innsbruck, Austria

# 44 Engineering quantum properties of molecular circuits with chemistry 09/07/2024 Masha Kamenetska

Boston University, Boston, MA, USA

# 45 Enumeration of spin-space groups: toward a complete description of symmetries of magnetic orders 15/07/2024 Chen Fang

Institute of Physics, Chinese Academy of Sciences, Beijing, China

## 46 Universal cold RNA phase transitions

17/07/2024 Felix Ritort Universitat de Barcelona, Spain

# 47 Pillar[5]arene scaffolds for the preparation of advanced materials and bioactive compounds

22/07/2024 Jean-François Nierengarten CNRS and University of Strasbourg, France

## 48 The role of 4f spin in single molecule magnets (SMMs) in generating Kondo states and Yu-Shiba-Rusinov states: insights from bis(phthalocyaninato)terbium(III) (TbPc<sub>2</sub>) adsorbed on superconductor Pb(111) surface 24/07/2024 Zhipeng Wang Tohoku University, Sendai, Japan

49 Non-reciprocity in superconductors - Josephson diode effect and beyond 29/07/2024 Christoph Strunk University of Regensburg, Germany

# 50 Seminar-I of internship students at DIPC 30/07/2024 Internship Students DIPC, Donostia/San Sebastián, Spain

# 51 Seminar-II of internship students at DIPC 30/08/2024 Internship Students DIPC, Donostia/San Sebastián, Spain

52 Achieving quantum utility for industrial applications in materials simulation 18/09/2024 Thomas Eckl Bosch Corporate Research, Germany

53 Flavin photocatalysis for the activation and delivery of metallodrugs 26/09/2024 Luca Salassa DIPC, Donostia/San Sebastián, Spain

# quantum magnets 30/09/2024 José Luis Lado Villanueva Aalto University, Espoo, Finland

# 14/10/2024 Yoshie Otake RIKEN, Wako, Japan

# 15/10/2024 Rik Broekhoven Delft University of Technology, The Netherlands

## 57 Multistability in guantum systems and related cavity QED experiments 18/10/2024 Peter Domokos HUN-REN Wigner Research Centre for Physics, Budapest, Hungary

# 58 Molecular assembly and reactivity triggered by Br-functional groups

24/10/2024 Lucia Vitali CFM, Donostia-San Sebastián, Spain

# 59 Rydberg atom arrays for quantum simulation, computation, and metrology 25/10/2024 Daniel Barredo Institut d'Optique-CNRS, CINN-CSIC, France and Spain

# 60 Leveraging machine learning for advanced materials discovery and electromagnetic applications 08/11/2024 Yang Hao Queen Mary University of London, UK

54 Hamiltonian learning, triplons, and high-order topological order in engineered nanoscale

55 RIKEN Accelerator-driven compact neutron systems, RANS project, and their capabilities

56 Efficient algorithm for dispersion of Yu-Shiba-Rusinov chains on a superconducting surface

#### 61 Coherent elastic neutrino-nucleus scattering in the standard model and beyond

14/11/2024 Valentina de Romeri Instituto de Física Corpuscular (IFIC), Paterna, Spain

# 62 Long-range entangling gates in constant depth using dynamic circuits 20/11/2024

Elisa Bäumer IBM, Germany

#### 63 In situ studies of hierarchical nucleation pathways in silicate and carbonate systems

22/11/2024 Jim De Yoreo Pacific Northwest National Laboratory (PNNL), Richland, WA and University of Washington, Seattle, WA, USA

# 64 Gravitational waves: the theorist's Swiss knife

27/11/2024 Mairi Sakellariadou King's College London, UK

#### 65 Landau-level mixing and SU(4) symmetry breaking in graphene

04/12/2024 Chunli Huang University of Kentucky, Lexington, KY, USA

#### 66 Quantum optics with organic molecules

10/12/2024 Diego Martín Cano IFIMAC, Universidad Autónoma de Madrid (UAM), Spain

#### 67 Anomalous quantum transport in fractal lattices

11/12/2024 Abel Rojo-Francàs Universitat de Barcelona, Spain

# 68 Understanding the modulators of tau amyloid aggregation pathways

12/12/2024 Yann Fichou Université Bordeaux/CNRS/Institut Européen de Chimie et Biologie, France

#### 69 Novel collective electronic phenomena in engineered 2D quantum materials 12/12/2024 Miguel Moreno Ugeda DIPC, Donostia/San Sebastán, Spain

## 1 Novel quantum dynamics with superconducting qubits 11/01/2024 Pedram Roushan Google Quantum AI, Santa Barbara, CA, USA

# 2 Bell inequalities: from curiosity to security 07/03/2024 Artur Ekert Merton College, University of Oxford, UK

## 3 Thinking outside the hypercube: RS and its implications 24/07/2024 Lisa Randall Harvard University, Cambridge, MA, USA

# 4 Do we really understand catalysis?

26/09/2024 Michele Parrinello Istituto Italiano di Tecnologia, Genoa, Italy

## 5 From inorganic photochemistry to molecular machines

27/11/2024 Jean-Pierre Sauvage ISIS, University of Strasbourg and CNRS, France

# Colloquia

L-Galaxies Workshop 2024... 14th European Symposium on Computing  $\pi$ -Conjug BioNEXT: 1st AEBIN Young Researchers Symposium. Anticancer Metal Drugs: New Developments and Fut Optics, Electronics and Magnetism in 2D Materials (C European South Atlantic Biophysics Congress – You XXI International Workshop on Quantum Atomic and III International Conference on Novel 2D Materials Explored via Scanning Probe Microscopy & Spectros Quantum Designer Physics 2024 (QDP2024)..... NanoNeuro 2024 .. Synthetic Electronic Quantum Matter (SELEQ)..... Quantum Phenomena in Multilayers and Heterostrue Challenges in Chemical Sensing with Graphene Deri BasQ Summer Course on Quantum Technologies... 7th Basque Quantum Science and Technology Work Transborder QuantumChemPhys Lab Workshop .....

#### Other Workshops

On-Surface Synthesis International Workshop (OSS20 International Quantum Matter Conference & Expo (C Artificial Intelligence for Advanced Materials (AI4AM2 XXXIX Reunión Bienal de la Real Sociedad Española o 9th International Doctoral Training Session "Frontiers

#### Scientific Meetings

2nd SPRING-DIPC Meeting	
PROTOS Kick-off Meeting	

# Workshops

	184
gated Compounds (CπC-14)	185
	186
ture Perspectives 2nd Edition (MDRUGMET)	187
OEM2D)	188
ng Scientist Seminar (ESAB-YSS)	. 190
d Molecular Tunneling Systems (QAMTS2024)	191
scopy (2DSPM)	193
	195
	197
	198
ictures (QPMH)	199
ivatives and 2D Materials (SENSE)	201
	. 202
<pre><shop (3rd="" ikur="" pre="" quantum="" workshop)<=""></shop></pre>	. 203
	204

QUANTUMatter 2024)	208
2024)	
de Física	213
s of Condensed Matter"	


# L-Galaxies Workshop 2024

#### January 22-24, 2024

Live streamed and in-person DIPC, Donostia/San Sebastián Shttps://lgalaxiespublicrelease.github.io/workshop2024.html

Organizing Committee Silvia Bonoli (DIPC, Ikerbasque) Rob Yates (University of Hertfordshire)

This meeting was aimed at discussing recent advancements and projects carried out with the galaxy evolution modeling code "L-Galaxies".



#### Invited Speakers

Nils Hoyer (DIPC, Spain) Rob Yates (University of Hertfordshire, UK) Markos Polkas (DIPC, Spain) Peter Thomas (Sussex, UK) David Izquierdo-Villalba (Universitá degli studi di Milano-Bicocca, Italy) Mohammadreza Ayromlou (Heidelberg University, Germany) Will Roper (Astronomy Centre, University of Sussex, UK) Akash Vani (MPA, Germany) Qingbo Ma (Guizhou Normal University, China) Qi Guo (NAOC, China) Daniele Spinoso (Department of Astronomy - Tsinghua University, China) Massimiliano Parente (SISSA, Italy) Jimi Harrold (University of Nottingham, UK) Matteo Bonetti (University of Milano-Bicocca, Italy) Julen Untzaga San Vicente (Institute of Space Sciences (ICE), Spain) Tong Su (National Astronomical Observatories, Chinese Academy of Sciences, China) Wenxiang Pei (NAOC, China) Jian Fu (Shanghai Astronomical Observatory, China)

# 14th European Symposium on Computing $\pi$ -Conjugated Compounds (C $\pi$ C-14)

#### February 8-9, 2024

Faculty of Education, Philosophy and Anthropology (HEFA I), Donostia/San Sebastián 𝔗 cpic14.dipc.org

Organizing Committee Claire Tonnelé (DIPC, Ikerbasque)

Since its beginning in 2010 in Valencia, the  $C\pi C$  symposium series has kept its original spirit of a convival gathering that offers an informal platform for the discussion of the latest research findings in the domain of  $\pi$ -conjugated systems. Topics encompass the fields of functional materials, photochemistry, biochemistry, theory and computation. In essence, it is a youthful, affordable, short and intimate event that aims to foster open and stimulating friendly discussions.

This year, the  $C\pi C$  symposium remained faithful to its spirit once again, promoting young scientists, local researchers, and rich and intense scientific exchange within this vibrant community.

This edition was sponsored by InSilibio and Springer Nature Group (Theoretical Chemistry Accounts journal) who awarded prizes for the best oral and poster contributions.



#### Invited Speakers

Elixabete Rezabal (UPV/EHU, Spain) Aran Garcia-Lekue (DIPC, Ikerbasque, Spain) Aurelio Mateo-Alonso (Polymat & UPV/EHU, Ikerbasque, Spain)



# BioNEXT: 1st AEBIN Young Researchers Symposium

#### March 14-15, 2024

Live streamed and in-person DIPC, Donostia/San Sebastián & https://bionext.dipc.org

# Organizing Committee Raphael de Paiva (DIPC, La Caixa) Ana C. Carrasco (DIPC) Douglas Hideki Nakahata (DIPC) María Jesús Morán (DIPC)

BioNEXT is a new initiative by Spanish Association for Bioinorganic Chemistry (AEBIN), complementing the "Bio" series of biannual in-person events organized by the society. The main purpose of BioNEXT was to serve as a venue to foment interaction between Spanish and international young researchers working in the field of bioinorganic and medicinal inorganic chemistry.

We organized three thematic sessions, including six invited talks and 13 talks from young researchers selected among the abstracts we received, covering the following themes:

- Frontiers in medicinal inorganic chemistry
- Biomolecular targets and mechanism of action of metallodrugs
- Intracellular catalysis

We also hosted eight flash presentations and a poster session with 79 posters.



#### Invited Speakers

Andrew Kellett (Dublin City University, Ireland) Caterina Ramogida (Simon Fraser University, Canada) Ramon Vilar (Imperial College London, UK) Jessica Rodríguez Villar (University of Santiago de Compostela) Gerard Roelfes (University of Groningen, Netherlands) James Coverdale (University of Birmingham, UK)

Together with our collaborator, ChemBioChem, we hosted a training session delivered by Dr. Ruben Ragg, editor-in-chief of the journal, and offered three prizes: one for the best oral communication by a young researcher, and two for the best posters.

BioNEXT received 264 attendees and presenters from 23 countries across Europe, the Americas, Africa, Asia and Oceania.

# Anticancer Metal Drugs: New Developments and Future Perspectives 2nd Edition (MDRUGMET)

May 15-17, 2024 DIPC, Donostia/San Sebastián

#### Organizing Committee

Luca Salassa (DIPC, Ikerbasque) Carlos Sanchez-Cano (DIPC, Ikerbasque) Raphael de Paiva (DIPC)

MDRUGMEET is an international scientific meeting, the first edition of which was held in Jerusalem (Israel) two years ago. In this second edition of the workshop, 25 prominent researchers from various European and Asian centers gathered to present unpublished results and discuss advancement in the field of medicinal inorganic chemistry. The unique format of the meeting helped to maximize interaction among researchers, thereby opening opportunities to consolidate existing collaborations and create new ones.



#### Invited Speakers

Angela Casini (Technical University of Munich, Germa Emilia Sicilia (University of Calabria, Italy) Vanesa Fernandez Moreira (University of Zaragoza, Sp Luisa Ronga (University of Pau et des Pays de l'Adour, Ana Pizarro (IMDEA Nanociencia, Spain) Petra Heffeter (Medical University of Wien, Austria) Giorgia Pastorin (National University of Singapore, Sing Dan Gibson (Hebrew University of Jerusalem, Israel) Luigi Messori (University of Florence, Italy) Ingo Ott (University of Braunschweig, Germany)

iany)	Nicola Margiotta (University of Bari, Italy)		
	José Ruiz (University of Murcia, Spain)		
ipain)	Gustavo Espino (University of Burgos, Spain)		
France)	Giampaolo Barone (University of Palermo, Italy)		
	Wee Han Ang (National University of Singapore, Singapore)		
	Patrick Gamez (University of Barcelona, Spain)		
gapore)	Samuel Meier-Menches (University of Wien, Austria)		
	Walter Berger (Medical University of Wien, Austria)		
	Christian Kowol (University of Wien, Austria)		
	Alessio Terenzi (University of Palermo, Italy)		

# Optics, Electronics and Magnetism in 2D Materials (OEM2D)

#### May 21-24, 2024

#### Organizing Committee

Garnett Bryant (Joint Quantum Institute, National Institute of Standards and Technology, University of Maryland) Thomas Weitz (Georg-August University Göttingen) Anna Seiler (Georg-August University Göttingen) Marta Pelc (Nicolaus Copernicus University in Toruń) Karolina Słowik (Nicolaus Copernicus University in Toruń) Andrés Ayuela (CSIC-UPV/EHU-MPC, DIPC) Mikel Arruabarrena (CFM-MPC, CSIC-UPV/EHU) Piotr Gładysz (Nicolaus Copernicus University in Toruń)

The OEM-2D International Conference aimed to establish and enhance collaborations between experts in the field, facilitating the exchange of ideas and research across several disciplines and serving as a platform for sharing perspectives and initiating collaborative projects.

By promoting a synergy of knowledge, the conference sought to accelerate progress and achieve significant advances in the areas of optics, electronics and magnetism, with special emphasis on graphene and other interesting 2D materials and nanostructures.

#### Supporting the next generation

The conference aimed to connect PhD students and postdoctoral researchers with the latest developments at the cutting edge of these fields. In this way it sought to bridge the gap between established researchers and emerging talent. It provided a valuable educational experience for young researchers through a combination of exhibition sessions and networking opportunities.



#### Invited Speakers

Eva Andrei (Rutgers University, USA) Jaroslav Fabian (University of Regensburg, Germany) Andrea Ferrari (Cambridge Graphene Center GC, UK) Gregory A. Fiete (Northeastern University of Boston, USA) Frank Koppens (ICFO, Spain) Stevan Nadj-Perge (Caltech, USA) Rick Silver (NIST, USA) Fan Zhang (UT Dallas, USA) Dario Bercioux (DIPC, Spain) Erez Berg (Weizmann Institute, Israel) Andres Castellanos (ICMM, Spain) Leonor Chico (Universidad Complutense, Spain) Joel Cox (University of Southern Denmark SDU, Denmark) Xiaodong Cui (University of Hong Kong, Hong Kong) Thomas Frederiksen (DIPC, Spain) Stephan Hofmann (Cambridge Graphene Centre GC, UK) Alexander Högele (Ludwig-Maximilians University of Munich, Germany) Shahal Ilani (Weizmann Institute, Israel) Włodzimierz Jaskólski (Nicolaus Copernicus University, Poland) Nicolas Lorente (CFM-CSIC, Spain) Paweł Machnikowski (Politechnika Wrocławska, Poland) Alejandro Manjavacas (Instituto de Óptica "Daza de Valdés" (IO-CSIC), Spain) Magdalena Margańska (University of Regensburg, Germany) Alexey Nikitin (DIPC, Ikerbasque, Spain) Hryhoriy Polshyn (Institute of Science and Technology Austria IST-A, Austria) Paweł Potasz (Nicolaus Copernicus University NCU, Poland) Lorenzo Del Re (Max Plank Institute for Solid State Research, Germany) Carsten Rockstuhl (Karlsruher Institut of Technology, Germany) Eli Zeldov (Weizmann Institute, Israel) Michał Zieliński (Nicolaus Copernicus University NCU, Poland)

# **European South Atlantic Biophysics Congress – Young** Scientist Seminar (ESAB-YSS)

June 4-5, 2024

DIPC, Donostia/San Sebastián Shttps://www.biophysicssansebastian2024.com/satellite-workshop

Organizing Committee

Aitziber L. Cortajarena (CIC biomaGUNE) David de Sancho (DIPC, UPV/EHU) Gabriel Ortega (CIC bioGUNE) Edurne Rujas (Biofisika, UPV/EHU) Aitor Manteca (CIC biomaGUNE)

The Young Scientist Seminar (ESAB-YSS) took place on June 4-5 at Donostia International Physics Center as a Satellite Workshop of the European South Atlantic Biophysics Congress. This workshop, designed to support early-stage researchers, brought together a vibrant community of 60 graduate students, postdoctoral researchers, and early-career scientists from various fields of biophysics.

The workshop sessions showcased the outstanding scientific work being conducted by the youngest members of the Spanish, Portuguese, and French biophysics communities. Each presentation was followed by lively discussions that encouraged the exchange of ideas and the exploration of new research directions.

Many attendees expressed their appreciation for the supportive environment and the chance to engage with leaders in the field. The organizing committee received positive feedback, particularly regarding the workshop's focus on young scientists.

#### Invited Speakers

Nunilo Cremades (Universidad de Zaragoza, Spain) Javier Fernández Martínez (Institute of Biofísika, Spain)

# XXI International Workshop on Quantum Atomic and Molecular Tunneling Systems (QAMTS2024)

June 16-21, 2024

Miramar Palace, Donostia/San Sebastián https://qamts2024.dipc.org

#### Organizing Committee

Ricardo Díez Muiño (DIPC, Ikerbasque) Antonio Fernández Ramos (Universidade de Santiago de Compostela) Salvador Miret Artés (Instituto de Física Fundamental CSIC)

Tunneling phenomena are of importance in a wide range of fields in the physical, chemical, biological and computational sciences. The series of Workshops on Quantum Atomic and Molecular Tunneling Systems has always been highly cross-disciplinary. It encompasses work on tunneling of protons and heavier species in gas and condensed phases, in general, including biological systems, chemical reactions, transport phenomena in solids and liquids and in systems of lower dimensionality.

The scientific program of QAMTS2024 included invited lectures as well as contributed talks and posters. There were scientific contributions on phenomena where atomic, molecular, or magnetic tunneling plays an important role, including not only processes in solids and matrices, but also organic and organometallic reactions in liquids, tunneling processes in clusters and nanoparticles, enzyme-catalyzed reactions, and some nontraditional emerging areas, this list being exemplary and non-exhaustive.



Octavio Roncero Villa (IFF, CSIC, Spain) Marta I. Hernández (IFF, CSIC, Spain) Alejandro González-Tudela (IFF, CSIC, Spain) John Ellis (Cavendish Lab., UK) Marco Sacchi (University of Surrey, UK) Jian Liu (University of Beijing, China) Chiara Aieta (University of Milano, Italy) Michele Ceotto (University of Milano, Italy) Jianshu Cao (MIT, USA) Sebastian Kozuck (University Ben-Gurion, Israel) Jeremy O. Richardson (ETH Zurich, Switzerland) Gunter Wichmann (ETH Zurich, Switzerland) Sotiris Xantheas (University of Washington, USA) Jon M. Matxain (UPV/EHU, Spain) Bo Chen (DIPC, Spain) Pavel Jelinek (Institut of Physics, Czech Republic) Karina Morgenstern (University of Bochum, Germany) Ion Errea (CFM- CSIC, Spain) Emilio Martínez-Núñez (Universidade de Santiago de Compostela, Spain) Katarzyna Swiderek (University Jaume I, Spain) Claudio M. Nunes (University of Coimbra, Portugal) Elena Jimenez (University of Castilla La Mancha, Spain) Robert McMahon (University of Wisconsin, USA) Franceso Paesani (University of California, USA) Zlatko Bacic (University of New York, USA) Ad van der Avoird (University of Nijmegen, Netherlands) Roberto Marquard (University of Strasbourg, France) Peter Saalfrank (University of Potsdam, Germany) Steven D. Schwartz (University of Arizona, USA) Wolfram Sander (University of Bochum, Germany) Sophya Garashchuk (University of South Carolina, USA) Alberto Lesarri (University of Valladolid, Spain) Micheline B. Sorey (University of Wisconsin, USA)

# III International Conference on Novel 2D Materials Explored via Scanning Probe Microscopy & Spectroscopy (2DSPM)

#### June 24-28, 2024

Miramar Palace, Donostia/San Sebastián *8* https://2dspm.dipc.org

Organizing Committee Miguel Moreno Ugeda (DIPC, Ikerbasque) Iván Brihuega (UAM, IFIMAC)

The III International Conference on Novel 2D Materials Explored via Scanning Probe Microscopy & Spectroscopy (2DSPM) aimed to bring together the scientific elite in the field of 2D materials to present and discuss the latest advancements in the field, offering innovative ideas as well as new methods to study the fundamental properties of these new materials at the atomic scale.

The conference program was particularly focused on scientists specializing in 2D materials studied through Scanning Probe Microscopy & Spectroscopy (SPM & SPS) methods. Scanning probe techniques are particularly suitable for the study of two-dimensional materials because, unlike most experimental techniques, they provide information about their atomic, electronic, and magnetic structure in real space with atomic resolution. For this reason, these techniques have recently taken on a fundamental role in the study of these new materials and, in general, in the field of Materials Science.

The conference also aimed to be a gathering point to discuss the current state of research in this area, focused on the search for new functional low-dimensional materials, with the participation of leading national and international researchers in the field as well as to promote and encourage interaction and collaboration between internationally renowned research groups in the field and theoretical and experimental groups working in the Basque Country.



Ali Yazdani (Princeton University, USA) Stevan Nadj-Perge (Caltech, USA) Jennifer Hofmann (Harvard University, USA) Stuart Parkin (Max Planck Institute, Germany) Shalal Alani (Weizmann Institute, Israel) Abhay Pasupathy (Columbia University, USA) Katharina J. Franke (Freie University, Germany) Francisco Guinea (DIPC, Spain) Eva Andrei (Rutgers University, USA) José Ignacio Pascual (CIC nanoGUNE, Spain) Haim Beidenkopf (Weizmann Institute, Israel) Roland Wiesendanger (University of Hamburg, Germany) Joseph Stroscio (NIST, USA) Maia G. Vergniory (Max Planck Institute, Germany) Joaquín Fernández-Rossier (INL Braga, Portugal) Peter Liljeroth (Aalto University, Finland) Roser Valentí (Goethe-University, Germany) Roman Fasel (EMPA, Switzerland) Nadine Hauptmann (Radboud University, The Netherlands) Sivan Refaeli-Abramson (Weizmann Institute, Israel) Lin He (Beijing Normal University, China) Feng Wang (UC Berkeley, USA)

# Quantum Designer Physics 2024 (QDP2024)

#### July 15-19, 2024

Miramar Palace, Donostia/San Sebastián https://qdp2024.dipc.org

#### Organizing Committee

Vitaly Golovach (CFM-UPV/EHU, DIPC, Ikerbasque) Francisco Guinea López (DIPC, IMDEA Nanoscience) Daniel Loss (University of Basel)

The workshop highlighted the 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 guantum materials and created a stimulating atmosphere for discussing physics on the marvelous sites of Donostia/San Sebastián. 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 topological and spin-based quantum computing with an outlook into the prominent future of guantum technologies. 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.



Shaffique Adam (National University of Singapore, Singapore) Yoichi Ando (University of Cologne, Germany) Christian Back (TU Munich, Germany) Sebastian Bergeret (CFM-CSIC, Spain) Andrei Bernevig (Princeton University, USA) Stefano Bosco (QuTech, The Netherlands) Sara Catalano (CFM-MPC, Spain) Silvano De Franceschi (CEA Grenoble, France) Olesia Dmytruk (CNRS, Institut Polytechnique de Paris, France) Jérôme Faist (ETH Zurich, Switzerland) Liang Fu (MIT, USA) Leonid Glazman (Yale University, USA) Shahal Ilani (Weizmann Institute of Science, Israel) Jelena Klinovaja (University of Basel, Switzerland) Roza Kotlyar (Intel, USA) Leo Kouwenhoven (TU Delft, The Netherlands) Henry Legg (University of Basel, Switzerland) Roman Lutchyn (Microsoft, USA) Allan MacDonald (University of Texas Austin, USA) Vladimir Manucharyan (EPFL, Switzerland) Pierre Pantaleon (IMDEA Madrid, Spain) Jeong Min (Jane) Park (MIT, USA) Stuart Parkin (MPI Halle, Germany) Nacho Pascual (Nanogune, Spain) Elsa Prada (ICMM-CSIC, Spain) Patrik Recher (TU Braunschweig, Germany) Pascal Simon (University Paris Saclay, France) Ady Stern (Weizman Institute, Israel) Dominik Zumbuhl (University of Basel, Switzerland)

# NanoNeuro 2024

#### July 20, 2024

Live streamed https://ntc.columbia.edu/nanoneuro-2024

#### Organizing Committee

Aitzol Garcia-Etxarri (DIPC, Ikerbasque) Rafael Yuste (Columbia University) Teresa Celaya (DIPC, Columbia University)

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.

NanoNeuro2024 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 supported by the Tianqiao and Chrissy Chen Institute.

The conference achieved its scientific objectives and was followed by a total 700 people, making it a great success of public as well.



Invited Speakers William Shih (Harvard University, USA) Bryan Roth (UNC, USA) Blanca del Rosal (RMIT, Australia) Pau Gorostiza (IBEC, Spain) José Antonio Garrido (ICN2, Spain) Katrin Willig (University of Augsburg, USA)

# Synthetic Electronic Quantum Matter (SELEQ)

August 28-30, 2024

Miramar Palace, Donostia/San Sebastián 𝔗 https://seleq24.dipc.org

#### Organizing Committee

Dario Bercioux (DIPC, Ikerbasque) Francois Dubin (CNRS) Tobias Grass (DIPC, Ikerbasque) Mohammad Hafezi (JQI, University of Maryland)

The SELEQ workshop brought together international scholars working on the challenge of controlling and manipulating electronic systems for the engineering of quantum correlations and many-body phases of real or synthetic matter. Experimental and theoretical experts presented the state-of-art related in scientific sessions dedicated to:

- Light-matter interactions in strongly correlated systems
- Excitons/exciton-polaritons
- Light-induced quantum phases
- Electronic guantum simulators
- Quantum dots
- Moiré systems



#### Invited Speakers

Eugene Demler (ETH Zurich, Switzerland) Sebastian Diehl (University of Cologne, Germany) Nathan Goldman (UL Bruxelles, Belgium) Tom Devereaux (Stanford University, USA) Ataç Imamoglu (ETH Zurich, Switzerland) Philip Kim (Harvard University, USA)

Camille Lagoin (CRHEA, CNRS, France) Jacqueline Bloch (University of Paris-Saclay, France) Cristiane Morais Smith (University of Utrecht, The Netherlands) Fabio Pistolesi (Université de Bordeaux, France) Marlou Slot (NIST, USA) Ingmar Swart (University of Utrecht, The Netherlands) Lieven Vandersypen (TU Delft, The Netherlands) Xiadong Xu (University of Washington, USA) Go Yusa (Tohoku University, Japan)

# **Quantum Phenomena in Multilayers and Heterostructures** (QPMH)

#### September 2-6, 2024

Miramar Palace, Donostia/San Sebastián https://qpmh.dipc.org

# Organizing Committee

Leni Bascones (ICMM-CSIC) Maria Gastiasoro (DIPC) Paula Mellado (Universidad Adolfo Ibañez) Ali Yazdani (Princeton University)

The aim of the workshop was to explore and discuss the correlated and topological phases of twisted and untwisted graphene and dichalcogenides multilayers, the properties of van der Waals magnets and interface superconductivity. Focus was given to the latest advances in the characterization, theory and ad-hoc engineering of new quantum states, as well as to breakthroughs in sensing and spectroscopic techniques to detect these novel states.

We list below some of the main scientific outcomes and achievements presented and discussed during the workshop:

- Novel evidence and techniques to detect Wigner crystals in graphene multilayers
- New techniques to detect topological edge states and to probe multilayers
- Novel measurements of fractional topological states in twisted dichalcogenides and penta-layer graphene • Evidence of very strong substrate and capping layer effect on the properties of multilayers from in-situ
- twisting techniques
- Novel theoretical proposals to detect the correlated states in twisted bilayer and trilayer graphene
- superconductors



• New insights of different mechanisms for exceeding the Pauli limit with spin-orbit coupling of interface



Another achievement that should be highlighted is the strong interaction and engagement that took place among attendees throughout the entire week, not only with many questions during and after the talks, but also during the lunch and coffee breaks.

Kaveh Ahadi (Ohio State University, USA) Monica Allen (UC San Diego, USA) Leon Balents (UC Santa Barbara, USA) Anand Bhattacharya (Argonne National Laboratory, USA) Silke Buehler-Paschen (Vienna University of Technology, Austria) María José Calderón (ICMM-CSIC, Spain) Andrey Chubukov (University of Minnesota, USA) Laura Classen (MPI-FKF Stuttgart, Germany) Santiago Grigera (Universidad Nacional de La Plata, Argentina) Shahal Ilani (Weizmann Institute of Science, Israel) Long Ju (Massachusetts Institute of Technology, USA) Raquel Queiroz (Columbia University, USA) Louk Rademaker (Geneva University, Switzerland) Rebeca Ribeiro-Palau (CNN-Saclay-CNRS, France) Carmen Rubio-Verdú (ICFO, Spain) Lucile Savary (CNRS, École Normale Supérieure de Lyon, France) Anna Seiler (ETH-Zurich, Switzerland) Miguel Ugeda (DIPC, Ikerbasque, Spain) Roser Valentí (Goethe Universität Frankfurt, Germany) Maia García-Vergniory (DIPC, Spain, MPI-CPfS, Germany) Xiaodong Xu (University of Washington, USA)

# Challenges in Chemical Sensing with Graphene Derivatives and 2D Materials (SENSE)

#### September 23-25, 2024

Miramar Palace, Donostia/San Sebastián & https://sense.dipc.org

Organizing Committee Martina Corso (CFM-CSIC) Aran Garcia-Lekue (DIPC, Ikerbasque) Aitor Mugarza (ICN2) Diego Peña (CiQUS) Dimas G. de Oteyza (CINN, CSIC-UNIOVI-PA)

Chemical sensors are part of modern society, finding broad applications in environmental and indoor monitoring, industrial safety, industrial chemical productions processes, pharmaceutical, food products, healthcare, security, etc. The workshop aimed to gather experts in the field of chemical sensing with two dimensional materials and graphene derivatives seeking for an efficient implementation of such materials in operating sensing devices and architectures. The three-day workshop, the first one of this kind, proved to be successful by creating a stimulating environment for exchange of ideas especially in gas and bio sensing. The workshop facilitated networking and collaboration opportunities among scientists from diverse research fields in experimental and theoretical physics, chemistry, engineering and materials science.



#### Invited Speakers

Cristina Africh (CNR-IOM, Italy) Alejandro Criado (Universidade da Coruña, Spain) Ganna (Anya) Gryn'ova (Heidelberg Institute for Theoretical Studies, Germany) Martina Lihter (Institute of Physics, Croatia) Michal Otyepka (CATRIN, Palacký University, Czech Republic) Celia Rogero (CFM- Spain) Paolo Samori (University of Strasbourg, France) Luigi Sangaletti (Università Cattolica del Sacro Cuore, Italy) Jose Angel Martin Gago (ICMM, Spain) Tao Wei (Friedrich Alexander University Erlangen-Nürnberg, Germany) Amaia Zurutuza (Graphenea, Spain)

# **BasQ Summer Course on Quantum Technologies**

September 9-11, 2024 Miramar Palace, Donostia/San Sebastián

Organizing Committee Javier Aizpurua (BasQ-DIPC, Ikerbasque) Igor Campillo (Euskampus Foundation)

Promoted by the BasQ initiative, Donostia International Physics Center (DIPC) and Euskampus Foundation, the Summer Course on Quantum Technologies was held as part of the Summer Courses organized by the Universidad del País Vasco / Euskal Herriko Unibertsitatea (UPV/EHU).

The event gathered experts from around the world, offering a unique opportunity to delve into the growing field of quantum technologies, which promises to transform sectors such as computing, telecommunications, and security, among many others.

The course featured a diverse program of lectures by renowned researchers and professionals in the field. Over the course of three days, topics such as quantum computing, quantum communications, quantum cryptography, and quantum sensing were addressed. Each of these areas was presented in an educational manner, demonstrating their real and potential impact on industry and society as a whole. Participants, including undergraduate, master's, and PhD students from various disciplines, as well as researchers and business representatives, were able to explore the disruptive potential of these innovations and their possible applications in the future.



#### Invited Speakers

Verónica Fernández Marmol (ITEFI-CSIC, Spain) Joana Fraxanet Morales (IBM Research, Spain) Yassine Hamoudi (LaBRI-CNRS, Université de Bordeaux, France) Eduardo Jacob Taquet (UPV/EHU, Spain) Nicolás Lorente Palacios (CFM-CSIC, Spain) Brahim Lounis (LP2N-Institut d'Optique, France) Gabriel Molina Terriza (CFM-MPC, Ikerbasque, Spain) Roman Orús (DIPC, Ikerbasque, Spain) Daniel Ramos (ICMM, Spain) Cristina Sanz (IBM Quantum, Spain) Martha Johanna Sepúlveda Flórez (Airbus Defence and Space)

# 7th Basque Quantum Science and Technology Workshop (3rd IKUR Quantum Workshop)

#### October 4, 2024

Camara de Comercio, Donostia/San Sebastián *8* https://giedke.dipc.org/eusqutech24.html

#### Organizing Committee

Géza Giedke (DIPC, Ikerbasque) Enrique Rico (UPV/EHU, Ikerbasque)

The meeting connected researchers from various research institutions of the Basque Country (BCAM, CFM, DIPC, Mondragon, Nanogune, Tecnun, UPV/EHU) and the Université de Bordeaux that work in the (broadly defined) field of quantum science and technology. It served as a platform to present recent results and enter into scientific exchange with colleagues, especially during the 2.5 hours poster session. In total, 14 talks and almost 40 posters were presented, meaning that almost two-thirds of all participants contributed to the program.



#### Invited Speakers

Pedro Crespo (Tecnun, Spain) Thomas Frederiksen (DIPC, Ikerbasque, Spain) Ruiyang Huang (Université de Bordeaux, France) Fabio Pistolesi (Université de Bordeaux, France) Manfred Mark (Universität Innsbruck, Austria) Géza Toth (UPV/EHU, Ikerbasque, Spain)

# Transborder QuantumChemPhys Lab Workshop

November 28-29, 2024

Bayonne, France  $\mathscr{O}$  https://dipc.ehu.eus/en/scientific-activities/workshops/transborder-quantumchemphys-lab-workshop

Organizing Committee Pascal Larregaray (ISM, CNRS - Université de Bordeaux) Ricardo Díez Muiño (DIPC, Ikerbasque)

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 November 28th-29th 2024, the QuantumChemPhys Lab organized a workshop in which recent activity on the topics of interest to the Lab was discussed. Forty-six scientists from the three institutions forming the QuantumChemPhys lab gathered in Bayonne. All PhD students and post-doctoral researchers that are 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 included in the program as well. This workshop contributed to the cohesiveness of the QuantumChemPhys lab, as well as building and developing new lines of research, in particular in the field of quantum computing.



#### Invited Speakers

Alejandro Rivero (Université de Lille, France) Raúl Bombín (ISM, CNRS - Université de Bordeaux, France) Juan Felipe Lew Yee (DIPC, Spain) Markel Ylla (UPV/EHU, Spain) Joan Grebòl-Tomàs (DIPC, Spain) Raidel Martín Barrios (ISM, CNRS - Université de Bordeaux, France) Duy Hoang Minh Nguyen (DIPC, Spain) Matt Hugget (ISM, CNRS - Université de Bordeaux, France) Nonia Vaguero (DIPC, Spain) Laura Viaud (ISM, CNRS - Université de Bordeaux, France) Angela Dellai (ISM, CNRS - Université de Bordeaux, France) Alicia Omist (DIPC, Spain) Antonio Cebreiro-Gallardo (DIPC, Spain) Janaarthana Babu Perumal Marisami (DIPC, Spain) Norhan Omar (ISM, CNRS - Université de Bordeaux, France) Antoine Patt (DIPC, Spain, ISM, CNRS - Université de Bordeaux, France) Moritz Frankerl (DIPC, Spain, LOMA, CNRS - Université de Bordeaux, France) Andrés Bejarano (DIPC, Spain, LOMA, CNRS - Université de Bordeaux, France) Josianne Owona (DIPC, Spain, ISM, CNRS - Université de Bordeaux, France) Isabella C. D. Merrit (ISM, CNRS - Université de Bordeaux, France) José Aarón Rodríguez-Jiménez (DIPC, Spain) Verónica Postils (ISM, CNRS - Université de Bordeaux, France; Catholic University of Louvain, Belgium) Roberto A. Boto (DIPC, Spain)

# Other Workshops

# On-Surface Synthesis International Workshop (OSS2024)

June 2-7, 2024 Hotel Eden Roc, Sant Feliu de Guixols & https://oss24.dipc.org

Organizing Committee Dimas G. de Oteyza (CINN, DIPC) Martina Corso (CFM, DIPC) Roman Fasel (EMPA)

On-surface synthesis, a surface-supported variation of organic chemistry most commonly performed under vacuum, 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.

Because this approach bridges across the fields of chemistry, physics and materials science, further involving engineering for the integration of these molecular materials in actual devices, the aim of this fifth 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. It has been a full success, bringing together 110 researchers from 17 different countries spread over various continents. Their respective expertise also spanned the whole range of disciplines involved in this field, overall promoting common approaches and collaborations that will in the end allow for the fastest and best possible advances in this promising research field.



#### Invited Speakers

Gabriela Borin-Barin (EMPA, Switzerland) Lifeng Chi (Soochow University, China) Joaquín Fernández-Rossier (International Iberian Nanotechnology Laboratory, Portugal) Felix Fischer (University of California at Berkeley, USA) Szymon Godlewski (Jagiellonian University, Poland) Pavel Jelinek (The Czech Academy of Sciences, Czech Republic) Jiong Lu (National University of Singapore, Singapore) Dolores Pérez (CIQUS, Universidade de Santiago de Compostela, Spain) Guillaume Schull (Institute of Physics and Chemistry of Materials of Strasbourg, France) Alexander Sinitskii (University of Nebraska-Lincoln, USA) Ping Yu (ShanghaiTech University, China) Junfa Zhu (University of Science and Technology of China, China)

# International Quantum Matter Conference & Expo (QUANTUMatter 2024)

May 7-10, 2024 Kursaal Congress Centre-Auditorium, Donostia/San Sebastian & https://www.quantumconf.eu/2024

#### Organizing Committee

Antonio Correia (Phantoms Foundation) Ricardo Muiño (DIPC, CFM-CSIC) Juan Jose Garcia-Ripoll (IFF-CSIC) Stephan Roche (ICREA / ICN2) Daniel Sanchez-Portal (CFM, Spain) Javier Aizpurua (CFM-CSIC, UPV/EHU, DIPC) Nacho Pascual (CIC nanoGUNE) Enrique Rico (UPV-EHU, Spain) Celia Rogero (CFM-CSIC, UPV/EHU)

The fourth edition of the Quantum Matter International Conference – QUANTUMatter 2024 (San Sebastian, 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.

This year, the Topological Matter Conference (TMC2024) joined forces with QUANTUMatter2024 featuring tutorials, specific workshops and speakers on topics such as topological insulators and Weyl semimetals, topological phononics and photonics, skyrmions, quantum metrology and more.





#### Invited Speakers

Ignacio Cirac (Max Planck Institute of Quantum Optics, Germany) Claudia Felser (Max Planck Institute for Chemical Physics of Solids, Germany) Leo Kouwenhoven (Delft University of Technology, The Netherlands) Michelle Simmons (University of New South Wales, Australia) Amir Yacoby (Harvard University, USA) Ana Asenjo-Garcia (Columbia University in the city of New York, USA) Philippe Bouyer (University of Amsterdam/Quantum Delta NL, The Netherlands) Deung-Jang Choi (CFM-CSIC, UPV/EHU, Spain) Jens Eisert (Freie Universität Berlin, Germany) Francesca Ferlaino (University of Innsbruck & IQOQI, Austria) Mohammad Hafezi (University of Maryland, USA) Angela Kou (University of Illinois Urbana-Champaign, USA) Anatoly Kulikov (ETH Zurich, Switzerland) Peter Lodahl (University of Copenhagen, Denmark) Yulia Maximenko (Colorado State Universtity, USA) Susanne Yelin (Harvard University, USA) Antonio Acin (ICFO, Spain) Audrey Bienfait (ENS Lyon, France) Frédéric Bonell (Spintec, France) Olivier Boulle (CEA, France) Jorge Casanova (UPV/EHU, Spain) Sonia Conesa Boj (TU Delft, The Netherlands) Joseph Dufouleur (IFW Dresden, Germany) Dmitri Efetov (LMU, Germany) Adolfo G. Grushin (Institut Néel / CNRS, France) Sophie Gueron (Université Paris Saclay - LPS, France) Matteo Ippoliti (The University of Texas at Austin, USA)

Karl Jansen (Deutsches Elektronen-Synchrotron DESY, Germany) Barbara Kraus (Technical University of Munich, Germany) Marie-Blandine Martin (CNRS-Thales, France) Nicola Poccia (IFW Dresden & University of Naples Federico II, Germany/Italy) Carmen Rubio Verdú (ICFO, Spain) Nitin Samarth (Penn State University, USA) Mikel Sanz (NQUIRE Center - UPV/EHU, Spain) Javad Shabani (New York University, USA) Matti Silveri (University of Oulu, Finland) Jairo Sinova (Johannes Gutenberg University Mainz, Germany) Magdalena Stobinska (Warsaw University, Poland) Sofia Vallecorsa (CERN, Switzerland) Visa Vesterinen (VTT, Finland) Silvia Zorzetti (Fermilab, USA) James S. Clarke (Intel, USA) Yonatan Cohen (Quantum Machines, Israel) Alexandre Dauphin (PASQAL, France) Artur Ekert (University of Oxford / Centre for Quantum Technologies, NUS, UK / Singapore) Jay M. Gambetta (IBM, USA) Pau Jorba (Kiutra, Germany) Yemliha Bilal Kalyoncu (Qblox BV, The Netherlands) Samira Nik (European Innovation Council (EIC), Belgium) Roman Orus (Multiverse Computing & DIPC, Spain) Claudius Riek (Zurich Instruments, Switzerland) Anurag Saha Roy (Qruise, Germany) Felice Francesco Tafuri (Keysight Technologies, USA) Jelena Trbovic (QuantrolOx, Finland) Ramon Aguado (ICMM-CSIC, Spain) Athanasios Dimoulas (NCSRD, Greece) Maia García Vergniory (Max Planck for Chemical Physics of Solids, DIPC, Germany/Spain) Tomas Jungwirth (Czech Academy of Sciences, Czech Republic)

# Artificial Intelligence for Advanced Materials (AI4AM2024)

#### July 2-4, 2024

Casa Convalescència, Barcelona Ahttps://www.ai4am.net/2024/index.php

#### Organizing Committee

Antonio Correia (Phantoms Foundation, Spain) Konstantin S. Novoselov (NUS / Institute for Functional Intelligent Materials, Singapore) Stephan Roche (ICREA/ICN2, Spain) Andrey Ustyuzhanin (Constructor, Germany) Ricardo Díez Muiño (DIPC, Ikerbasque, Spain) Concepción Narros Hernández (Phantoms Foundation, Spain) Joaquín Gaspar Ramón-Laca Maderal (Phantoms Foundation, Spain) Jose Luis Roldán (Phantoms Foundation, Spain)

Al4AM2024 was a cross-disciplinary international event that joined top experts from industry and research institutions utilizing Artificial Intelligence, including machine learning, deep learning, and neural networks. The event aimed to enhance discoveries in materials science by refining automated designs for both structural and electronic material models in engineering. It focused on improving interoperability among material databases and reverse material engineering. This platform offers experts an opportunity to delve into the latest innovations, discuss practical challenges, and share solutions in applying Al for groundbreaking advancements in material science and engineering. It covers targeted applications in electronics, composites, energy, (bio) medicine, quantum computing, and related fields. This inaugural edition set the groundwork for a series of conferences dedicated to this theme, fostering networking, collaboration, and industrial partnerships.





Kostya Novoselov (NUS, Singapore) Amanda Barnard (Australian National University, Australia) Sergei V. Kalinin (UT Knoxville and Pacific Northwest National Laboratory, USA) Karsten Reuter (Max-Planck-Gesellschaft, Germany) Marin Soljacic (MIT, USA) Anatole von Lilienfeld (University of Toronto, Canada) Maite Alducin (CFM, Spain) Juan Carrasquilla Alvarez (ETH Zurich, Switzerland) Bingqing Cheng (UC Berkeley, USA) Kamal Choudhary (NIST, USA) Giulia Cisotto (University of Milan-Bicocca, Italy) Gabor Csanyi (University of Cambridge, UK) Gianaurelio Cuniberti (TU Dresden, Germany) Volker Deringer (University of Oxford, UK) Andrea Ferrari (Cambridge Graphene Centre / University of Cambridge, UK) Kedar Hippalgaonkar NTU, Singapore) Boris Kozinsky (Harvard University, USA) Nicola Marzari (EPFL, Switzerland) Kostya Novoselov (NUS, Singapore) Wolfgang Wenzel (Karlsruhe Institute of Technology, Germany)

# XXXIX Reunión Bienal de la Real Sociedad Española de Física (RSEF)

#### July 15-19, 2024

Musikene and School of Engineering of Gipuzkoa, Donostia/San Sebastián Shttps://bienalfisica.org/en/home

#### Organizing Committee

Jenaro Guisasola (UPV/EHU) Ion Errea (CFM-UPV/EHU) Idoia G. Gurtubay (UPV/EHU) Josu M. Igartua (UPV/EHU) Mikel Sanz (UPV/EHU, Ikerbasque) Mikel Garmendia (UPV/EHU)

The RSEF Biennial served as a platform for the exchange of knowledge, the presentation of new research and the discussion of developments in various fields of physics. It was probably the largest event held in the Spanish state in the field of physics, covering all its fields from particle physics, biomedical physics and solid state physics, to physics education. It offered a unique platform for professionals, researchers, educators and students to participate in scientific discourse and establish new collaboration networks.

The main objectives have been the following:

- findings in various subfields
- share resources and knowledge



• Dissemination of Scientific Research. The biennial facilitates the presentation of cutting-edge research

 Promotion of Collaboration. The event promotes networking and collaboration opportunities between physicists from different institutions and countries, which is essential to develop joint research projects and

• Education and Dissemination. The biennial emphasizes the importance of education and public outreach, including sessions designed to improve the teaching of physics and promote public understanding of science

• Recognition of Excellence. During the biennial, prizes and recognitions are awarded, such as the prizes for the best doctoral theses of the RSEF+EPJ, highlighting significant achievements within the community
#### Invited Speakers

Sayeef Salahuddin (University of California Berkeley, USA) Clivia, Sotomayor Torres (ICN2, Portugal) Roberto, Gómez Calvet (European University of Valencia, Spain) Francisco Savall (IES Veles e Vents, Spain) José Luis, Sánchez Gómez (University of León, Spain) Yolanda Prezado (Institut Curie, France) Ursulla Keller (ETH Zurich, Switzerland) Olga Smirnova (Max Born Institute, Berlin) Juan Ignacio Cirac (Max Planck Institute for Quantum Optics, Germany) Javier Aizpurua (DIPC, Spain) Ricardo Díez Muiño (DIPC, Spain) Jorge Mira (University of Santiago de Compostela, Spain) Alessandra Buonanno (Max Planck Institute for Gravitational Physics, Germany) Jonathan Home (ETH Zurich, Switzerland) Jorge Méndez (University of La Laguna Tenerife, Spain) Irene Abril (University of Cambridge, Spain) Verónica Sanz (University of Valencia, Spain) Inmaculada Pérez Pérez (Friedrich Schiller University Jena, Germany) Pedro Miguel Echenique (UPV/EHU, Spain) Itziar Otegui (CIC NanoGUNE, Spain) Jorge Bravo-Abad (Universidad Autónoma de Madrid, Spain) Claudio Zeni (Cambridge University, UK)

# 9th International Doctoral Training Session "Frontiers of Condensed Matter"

#### September 16-27, 2024

École de Physique des Houches, France Shttps://www.houches-school-physics.com/program/program-2024/ frontiers-of-condensed-matter-1305548.kjsp

#### Organizing Committee

Sebastian Bergeret (DIPC, CFM/CSIC) Julia Meyer (Université Grenoble Alpes) Jörg Schmalian (Karlsruhe Institute of Technology) Christian Schönenberger (Swiss Nanoscience Institute, University of Basel) Gary Steele (TU Delft)

Frontiers of Condensed Matter offered final year master's students and junior PhD students a high-level training program in the general area of condensed matter physics. The session consisted of a lecture series on topics such as Quantum Transport, Topological Phases, Superconductivity, and Quantum Information - complemented by more specialized pedagogical seminars on timely topics as well as poster sessions and discussion forums. This was the 9th event in a series of doctoral training sessions organized since 2010.



#### Invited Speakers

Carlo Beenakker (Leiden, The Netherlands) Vidya Madhavan (Urbana-Champaign, USA) Sophie Guéron (University of Paris-Saclay, France) Adolfo Grushin (Institut Néel Grenoble, France) Anja Metelmann (Institute for Theoretical Condensed Matter Physics Karlsruhe, Germany) Zaki Leghtas (Mines Paris, France) Natalia Chepiga (Delft University of Technology, The Netherlands) Silvano De Francheschi (CEA Grenoble, France) Maria Gastiasoro (DIPC, Spain) Yaroslav Herasymenko (Delft University of Technology, The Netherlands) Christophe Mora (Université de Paris, France) Silke Paschen (Vienna University of Technology, Austria) Marta Pita-Vidal (IBM Research Zurich, Switzerland)

## Scientific meetings

## 2nd SPRING-DIPC Meeting

February 26-28, 2024 Doneztebe/Santesteban, Navarra

The second SPRING-DIPC MEETING brought together researchers from diverse disciplines, so as to create a fertile ground for academic exchange, promoting scientific discussion in an overarching atmosphere of open dialogue and collaboration.



Meeting attendants Thomas Frederiksen (DIPC, Ikerbasque, Spain) Tobias Grass (DIPC, Ikerbasque, Spain) Geza Giedke (DIPC, Ikerbasque, Spain) Natxo Pascual (CIC nanoGUNE, Ikerbasque, Spain) Nico Leumer (DIPC, Spain) Roberto Alvarez Boto (DIPC, Spain) Moritz Frankerl (DIPC, Spain) Martín Irizar (DIPC, Spain) Shayan Edalatmanesh (DIPC, Spain) Talat Rahman (University of Central Florida, Orlando, USA) Matt Hugget (Collège Sciences et Technologies - Université de Bordeaux, France) Sourav Biswas (DIPC, Spain) Alicia Omist Galvez (DIPC, Spain) Sofía Sanz Wuhl (Materials Physics Center CFM-CSIC, Spain) Ricardo Ortiz (DIPC, Spain) Daniel García (DIPC, Spain) Daniel Sánchez Portal (Materials Physics Center CFM-CSIC, Spain)

## **PROTOS Kick-off meeting**

July 14-16, 2024 Olarain, Donostia/San Sebastián

The first gathering of the ERC-PROTOS synergy project focused on establishing the working profile for the upcoming years. Both scientific and administrative key goals were discussed and stablished.



Meeting attendants Juan Manuel Garcia (DIPC) Christian Jenewein (DIPC) Olatz Leis (DIPC) Mikel Abadia (DIPC) Wolfgang Bach (UBremen) Mark van Zuilen (Naturalis) Denis Gebauer (LUH) Stefan Lalonde (CNRS) Isaac Rodriguez (INPT) Sebastien Teychene (INPT) Fermín Otálora (CSIC)

#### DIPC Schools

Photo- and Electrocatalysis at the Atomic Scale (PE Nanothechnology Meets Quantum Information (Na Topological Matter School (TMS2024)...

#### DIPC Courses

Excited State Charge Dynamics and Optical Response of 2D Materials: Interplay Excitons and Phonons..... Innovations in Spintronics, Quantum Technologies

#### Transferable Skills Courses

First and Second Edition: Oral Presentation Skills Tr Generative AI: Useful Tools or Expensive Toys?..... Balancing Science and Self: Advanced Soft Skills for

Theses..

# Higher Education

ECAS 2024)	
lanoQl'24)	

							 	 	 . 225
5 6	and	Adv	ance	d Ele	ctror	nics.	 	 	 . 226

raining	227
	228
or Pl's	229

	30
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## **DIPC Schools**

## Photo- and Electrocatalysis at the Atomic Scale (PECAS 2024)

May 6-9, 2024 Faculty of Chemistry (UPV/EHU), Donostia/San Sebastián & https://pecas2024.dipc.org

Organizing Committee CAT&SCALE network Sara Barja (CFM-UPV/EHU, DIPC, Ikerbasque) Nuria López (ICIQ) José Ramón Galán (ICIQ) Sixto Giménez (INAM-UJI) Irene Palacio (ESISNA-ICMM) David Écija (IMDEA Nanoscience) Jordi Arbiol (ICN2) Pelayo García de Arquer (ICFO) Maria Escudero-Escribano (ICN2) María Giménez (CiQUS)

As in previous editions, PECAS 2024 was aimed at promoting interdisciplinary discussions among scientists in the fields of materials science and photoelectrochemistry, as well as the presentation of new results, ideas, and methods to understand the catalyst-electrolyte interface at the atomic level.

The program began with a two-day school featuring introductory lectures on surface science, electrochemistry, and theoretical methods. These lectures were specifically designed to introduce master's and graduate students in Chemistry and/or Physics to the topics covered in PECAS 2024. After the school, PECAS 2024 continued with a two-day workshop, including postgraduate-level seminars in surface science and electrochemistry. Hands-on experiments in NAP-XPS, STM/nc-AFM, and electrochemistry were also conducted to introduce participants to key surface science tools.



#### Invited Speakers

Herbert Over (Justus Liebig University, Germany) Julia Kunze-Liebhäuser (University of Innsbruck, Austria) Hendrik Bluhm (Fritz Haber Institute of the Max Planck Society, Germany) Paramarconi Rodriguez (CIC energiGUNE, Spain) Karoliina Honkala (University of Jyväskylä, Finland) Nùria López (Institute of Chemical Research of Catalonia ICIQ, Spain) Andrea Auer (University of Innsbruck, Austria) Pelayo García de Arquer (ICFO, Spain) Marko Melander (University of Jyväskylä, Finland) Juan Jesús Velasco Vélez (Cells ALBA, Spain) María del Carmen Giménez-López (CiQUS, Spain)

## Nanotechnology Meets Quantum Information (NanoQI'24)

#### July 22-25, 2024

Miramar Palace, Donostia/San Sebastián *&* http://nanoqi.dipc.org

## Organizing Committee Géza Giedke (DIPC, Ikerbasque) Alejandro Gonzalez-Tudela (IFF CSIC, Madrid) Atac Imamoglu (ETH Zurich)

The speakers highlighted various active research directions in the area where quantum information and nanotechnology meet, ranging from the design of naturally protected qubits to quantum enhanced time-keeping and quantum-enabled communication protocols on the theory side to the implementation of coherent quantum dynamics and QIP protocols in diverse platforms (semiconductor quantum dots, quantum emitters in chiral waveguides, atomic spins on insulating or superconduction surfaces, magnons, two-dimensional materials, or cold atoms in optical tweezers. More than two thirds of the students presented a poster and actively discussed their work throughout the poster session and coffee breaks. They were also very active and inquisitive in all the lectures, making this the most successful edition of NanoQI so far. On the other hand, it was the least successful in terms of total attendance.

By their participation, the participants gained a broader and deeper knowledge of the covered fields and the methods used. In addition, they had the opportunity to get to know and network with their colleagues.





#### Invited Speakers

Jason Alicea (Caltech, USA) Daniel Barredo (CINN-CSIC, El Entrego, Spain) Harry Buhrman (QuSoft, The Netherlands and Quantinuum, UK) Deung-Jang Choi (CFM-CSIC, Ikerbasque, Spain) Francisco Guinea (IMDEA, DIPC, Spain) Klemens Hammerer (University of Hannover, Germany) Atac Imamoglu (ETH Zurich, Switzerland) Silvia Kusminskiy (RWTH Aachen, Germany) Hannes Pichler (University of Innsbruck, IQOQI, Austria) Seigo Tarucha (RIKEN, Japan)

## **Topological Matter School (TMS2024)**

August 19-23, 2024

Miramar Palace, Donostia/San Sebastián 𝔗 https://tms.dipc.org

#### Organizing Committee

Maia G. Vergniory (DIPC, Max Planck for Chemical Physics of Solids) Reyes Calvo (Universidad de Alicante, Spain) Santiago Blanco-Canosa (DIPC, Ikerbasque) Adolfo Grushin (Institut NEEL - CNRS) Alexander Altland (University of Cologne, Germany) Julen Ibañez-Azpiroz (Materials Physics Center, Ikerbasque)

In this year's edition the topic was topologically correlated flat bands. Flat band materials offer a platform for enhancing correlation effects, rendering them an area of significant current interest. They present exceptional opportunities for exploring topology in correlated settings and correlation physics enriched by topology. Recent experiments on correlated kagome metals and Moiré systems have unveiled evidence of peculiar behaviors, including strange-metal characteristics, charge density waves, nematic orders, and fractional Chern insulators within flat-band materials. Throughout this school, our objective was to delve into the study of flat bands and these systems, as well as the intriguing physical phenomena they manifest, under the guidance of world-leading experts.





Invited Speakers Andrei Bernevig (Princeton University, USA) Alexander Altland (University of Cologne, Germany) Ming Yi (Rice University, USA) Leni Bascones (CSIC, Spain) Erez Berg (Weizmann Institute, Israel) Stephen Wilson (University of Santa Barbara, USA) Zhida Song (Peking University, China) Nicolas Regnault (CNRS, France) Yves Hon Kwan (Princeton University, USA) Carmen Rubio-Verdú (ICFO, Spain) Vidya Madhavan (University of Illinois, USA) Allan MacDonald (University of Austin, USA) Päivi Törmä (Aalto University, Finland)

## **DIPC** Courses

## Excited State Charge Dynamics and Optical Response of 2D Materials: Interplay Excitons and Phonons

February 29 - March 26, 2024 DIPC Auditorium, Donostia/San Sebastián

#### Talat S. Rahman

Department of Physics, University of Central Florida, Orlando, Florida

A striking feature of 2D transition metal dichalcogenides (TMDs) is the large exciton binding energy, which together with strong interactions between the electrons, holes, excitons, and phonons, promise the potential for applications in energy harvesting. These strong nonlinearities may be reflected in the characteristics of the resulting photocurrent and the emission spectra, for example, through high harmonic generation. In this talk, after attributing the experimentally observed anomalous optical band gap energy redshift, with increasing isotope mass, in single layer MoS<sub>2</sub>, to strong exciton-phonon coupling, we turned to phononassisted charge and exciton dynamics and photoluminescence in single layer and bilayer MoS<sub>2</sub> and WSe<sub>2</sub>. Shown, through application of time dependent density functional theory (TDDFT) and many-body theory, the (momentum-resolved) intra- and inter-valley dynamics, and photoluminescence in these 2D TMDs is a result of complex collective response involving the free charges, bright and dark excitons, and phonons. Our conclusions are validated by experimental data where available.

## **Innovations in Spintronics, Quantum Technologies** and Advanced Electronics

July 9-18, 2024 DIPC Auditorium, Donostia/San Sebastián

#### Stephan Roche

Institut Català de Nanociència i Nanotecnologia (ICN2), Barcelona, Spain

#### This DIPC Course was composed of four lectures:

#### LECTURE 1 Ten Years of 2D Materials based Spintronics Research: Highlights and Future

Objective: Present an historical perspective of why graphene and other two-dimensional materials have been anticipated as enabling materials to revolutionize the transfer, storage, and processing of spin information in the context of spintronic applications. This bird's-eye view emphasized the various milestones unique capability of these materials for manipulating spin degree of freedom at room temperature and over unprecedented length scales. Beyond the efforts to move from lab to fab and the current state-of-the-art in the research at high technology readiness level, the prospect for spin logics or other spin-dependent technologies were also addressed.

#### LECTURE 2 Linear scaling quantum transport methodologies applied to Topological Matter

Objective: This lecture introduced linear scaling transport methodologies which are the only possible tool giving access to complex quantum transport physics in realistic models of disordered systems contained up to a billion atoms. By connecting DFT approaches to tight-binding parametrization, the elaborate models can capture both perturbative and nonperturbative effects of a variety of disorder sources, and give access to resonant transport, weak (anti)-localization, strong localization regimes as well as topological phenomena (quantum Hall effects and so on). The combination of bulk with multiterminal transport approaches was also shown key to solve controversial claims of topological physics in nontrivial heterostructures.

#### LECTURE 3 Topological Spin Transport & Entanglement in Quantum Materials

Objective: This lecture presented spin transport phenomena related with the emergence of nontrivial spin textures in topological materials with low symmetries. It was shown that persistence spin textures result in canted spin Hall and canted Quantum spin Hall effects in monolayer transition metal dichalcogenides (TMDs), offering a novel platform for manipulating spin degree of freedom in topological phases, opening some road to topological spintronics. The spin-orbit torque phenomenon was also discussed in Janus TMDs, with theoretical predictions showing unprecedented performances.

LECTURE 4 Exploring properties and applications of amorphous 2D materials using Artificial Intelligence

Objective: This lecture focused on the presentation of machine-learning based models of amorphous materials, which enable the access to quantitative predictions of their properties. Contrary to initial expectations at first sight, amorphous materials are offering novel types of improvement of a variety of properties for coating applications (anticorrosion, barrier to migration), interconnects (ultralow dielectric coefficient) or neuromorphic computing (memristive devices). Artificial Intelligence was shown to be key for future breakthroughs in these fields.

#### 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. Organized by Aitzol García-Etxarri (DIPC, Ikerbasque) and Gustavo A. Schwartz Pomeraniec (DIPC, CFM-CSIC) DIPC develops a full program covering issues like stress management, time and career management or transformative leadership. 40 researchers joined these courses in 2024.

# First and Second Edition: Oral Presentation Skills Training

### May 14, 21 and 28, June 7, 13 and 21, 2024 DIPC Josebe Olarra Auditorium, Donostia/San Sebastián

#### Sofía Facal

Skills for Science and Industry

The ability to communicate complex topics in a clear and efficient way is a key skill in the academic field, as the success of bright ideas, great initiatives and promising projects can depend significantly on how they are presented.

In this training the participants further develop their skills in preparing and delivering top quality scientific presentations, as well as in communicating with audiences of different levels of expertise in their field.

#### SESSION 1 Before the Presentation

- Understanding your audience
- Structuring your message
- Designing effective slides
- Timing your talk
- What do people care most about scientific talks

#### SESSION 2 During the Presentation

- Body language
- Voice and articulation
- Anti-nervousness program
- Stress management

#### SESSION 3 After the Presentation

- Delivering the 10 mins talk you have prepared
- Constructive feedback
- Techniques for a Successful Q&A session
- Designing and presenting scientific posters

## Generative AI: Useful Tools or Expensive Toys?

#### June 13, 2024

DIPC Josebe Olarra Auditorium, Donostia/San Sebastián

#### Tim Smithers

The purpose of this course was to examine the benefits and risks of Generative AI systems, such as ChatGPT, in common research practices.

Generative AI systems now cover text, sound (speech and music), image, and video, generation, and combinations of these. A basic understanding of how these systems work and what they really do is needed to be able to judge well if and how they may be used in professional research practices, such as preparing research publications, funding proposals, presentations and talks, and computer code. Understanding how ChatGPT works and how the so-called Large Language Model (LLM) inside it is built does provide a good basis for deciding how and when good use might be made of any of the Generative Al systems. The important ethical issues and hazards raised by using ChatGPT in research practices are also common across the other kinds of Generative AI systems.

#### Outline of the course:

A few words on using tools in purposeful activities (and using toys). Some terminological explanations to get started with How to build a Large Language Model (a cartoon sketch). What does ChatGPT really do (it doesn't do writing!). A look at what happens when we try to use ChatGPT. Some ethical issues and hazards of using Generative AI systems. Discussion and Questions.

# Balancing Science and Self: Advanced Soft Skills for PI's

#### October 16 and 23, 2024

CFM Auditorium, Donostia/San Sebastián

#### October 30, 2024

DIPC Josebe Olarra Auditorium, Donostia/San Sebastián

#### Sofía Facal

Skills for Science and Industry

The training program "Balancing Science and Self: Advanced Soft Skills for PIs" was designed to address the need for soft skills development among Principal Investigators (PIs). The role of a PI goes beyond technical expertise, as they are responsible for shaping the direction of their research teams and fostering a good working culture.

Stress management, effective communication, emotional intelligence, and interpersonal skills form the backbone of successful leadership, creating a positive and collaborative environment where team members feel valued and supported. This training recognized the importance of soft skills and provided tools, the necessary self-reflection for each PI to lead, influence, and nurture within their own unique style, their research groups.

This training program was designed for researchers who seek to improve the art of balancing their scientific career with personal well-being. Through interactive sessions, they reflected on advanced soft skills, discovered effective stress management techniques, and explored strategies to achieve a healthy work-life balance. Our goal was to foster resilient, mindful, and highly effective leaders in the research community.

#### SESSION 1 Mastering Self-Awareness and Mindfulness in Leadership

- and team dynamics
- and improve decision-making
- fostering a supportive and productive research environment

#### SESSION 2 Effective Stress Management for Research Leaders

- Tools to recognize and address common stressors
- A toolkit of stress reduction methods, including time management, prioritization, and relaxation techniques
- and well-being among team members

#### SESSION 3 Advanced Communication and Conflict Resolution

- within diverse research teams
- promotes growth, understanding, and cohesion within the team

• Techniques to increase self-awareness and understand its impact on leadership style

Practical mindfulness exercises for busy schedules to enhance focus, reduce stress,

Strategies to manage emotions and understand the emotional needs of team members,

• Strategies to cultivate a research environment that promotes mental health, resilience,

Understanding the importance of balance for long-term productivity and personal well-being

- Communication Skills: Advanced strategies for clear, empathetic, and effective communication

Conflict Resolution: Approaches to resolving disagreements and conflicts in a way that

### Theses

## Fundamentals of nano-optics in hyperbolic van der Waals materials. Gonzalo Álvarez Pérez 24/01/2024 Supervisors: Pablo Alonso González and Alexey Nikitin

Probing nanoscale light-matter interactions with fast electrons and near-field optical probes. Carlos Alberto Maciel Escudero 09/02/2024 Supervisors: Javier Aizpurua Iriazabal and Rainer Hillenbrand

Quantum simulation of two-dimensional electronic lattices. Miguel Ángel Jiménez Herrera 07/03/2024 Supervisors: Dario Bercioux and Aitzol García Etxarri

Development, implementation and applications of hybrid quantum chemistry models. José Aarón Rodríguez Jiménez 15/03/2024 Supervisors: David Casanova Casas and Eduard Matito Gras

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