DIPC 2019

Donostia International Physics Center

ON THE COVER SEEING THE REACTIONS

Surface-supported chemistry under vacuum is an attractive complement to conventional chemistry, since the vacuum environment and the surface confinement impose boundary conditions that often drive the chemical reactions along unprecedented routes. In addition, it allows the performing of single-molecule studies of reactants and products, including the visualization of their covalent structure. As an example, the cyclo-trimerization product of 2-ethynylpyrene is pictured on the cover as observed with a scanning tunneling microscope at 4.3 K with the help of a CO-functionalized probe.

Cover image and diagram: J. Lawrence, M.S.G. Mohammed, A. Berdonces-Layunta and D.G. de Oteyza

2019

DIPC ACTIVITY REPORT

At DIPC, we trust

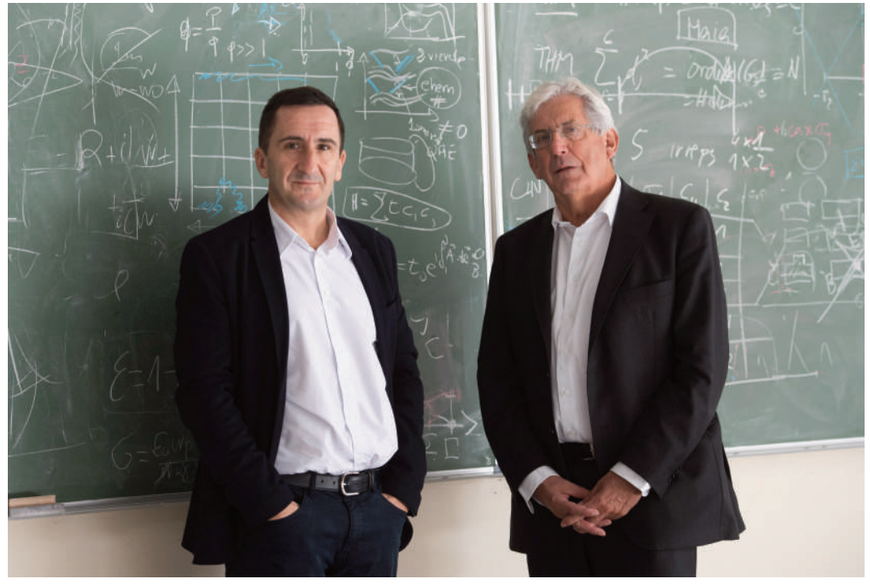
Donostia International Physics Center (DIPC) is a research center opened in the year 2000. DIPC's mission is to perform and catalyze research in physics and related disciplines, as well as diffusing scientific culture in society. DIPC gathers public institutions (Basque Government, Gipuzkoa Provincial Council, San Sebastian City Council, and University of the Basque Country) and private companies (currently Kutxa, CAF, Telefónica, and EDP) in jointly pursuing the development of science.

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.**

DIPC is an agile center that runs under a flexible and autonomous form of management and in which researchers are a top priority. DIPC stands as an international hub between the local community of researchers and a worldwide network of scientists. A constant flow of new ideas is fostered through a strong program of visiting researchers.

One of the major roles of any organization is to provide the necessary grounding for its members to develop their full potential. This is especially true for research centers. Science is a creative and time-consuming activity that requires a congenial and intellectually stimulating atmosphere to flourish. DIPC hosts scientists who are knowledgeable, curious, and passionate about their research. Besides providing the material means and an inspiring environment, DIPC offers two essential elements to the scientists: freedom and trust. Freedom to select their research topics and trust to tackle risks as a natural part of the discovery endeavor.

Scientists at DIPC make use of granted freedom and trust to perform research on condensed matter theory, advanced materials, surfaces and interfaces, photonics, plasmonics, quantum information, quantum technologies, polymers, soft matter, biofunctional nanosystems, computational chemistry, experimental particle physics, computational cosmology, and neutronics, to name just a few of the topics active in the center. The diversity of DIPC's research lines creates a lively scientific ambience and provides fertile ground for interdisciplinary projects.



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

As an important part of our mission, we embrace the responsibility of sharing science. DIPC develops a broad outreach program that is detailed in this report. In 2019, we celebrated a new edition of our triennial scientific festival Passion for Knowledge. The program included activities for students, music, videos, humor, poetry and the very popular series of plenary lectures addressed to a general audience and delivered by high-profile scholars, including six Nobel Laureates. Once more, we were delighted to see the enthusiastic response of the public and the curiosity and interest they showed for science. The Victoria Eugenia Theater, historical venue of cultural life in Donostia, was filled for six days to attend our sessions. Similar excitement arose in the Guggenheim Museum (Bilbao) and in Baluarte (Pamplona).

At DIPC, we trust our scientists and we trust and invest in the future. Science and education are pillars of human progress, not only economic and technological progress, but cultural and social as well. The work that we do at DIPC contributes to the generation of knowledge, the education of the citizens, and to the promotion of critical thinking. There are many challenges lying ahead in this increasingly complex and interconnected world. We are aware of some of them (sustainable development, inequality...) but we are still ignorant about others that will unexpectedly emerge. Science will be a necessary instrument to confront them and transform the world for the better. At DIPC, we trust in science. ■

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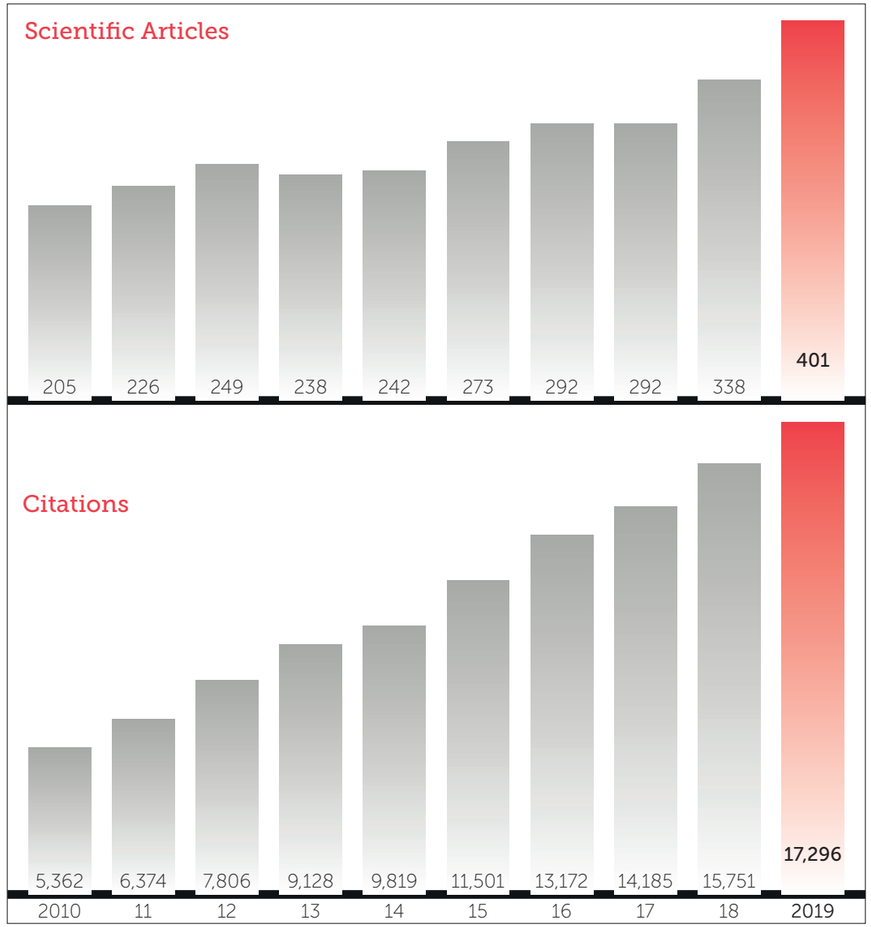
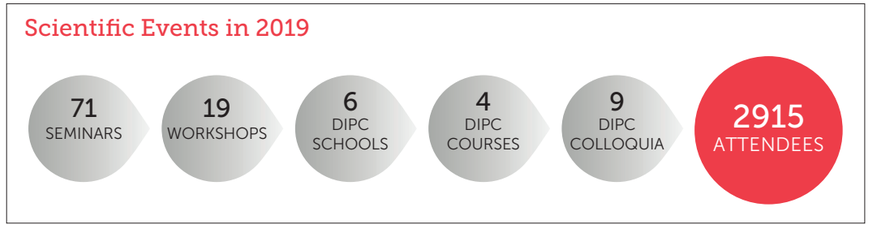
Research Activity at a Glance

DIPC's scientific production and international impact continues to increase. During the last 21 years, the center has published a total of **4,070 ISI publications** and has received more than **133,048 citations**. In 2019, **401 scientific articles** were published, up from 338 in 2018 and 292 in 2017.



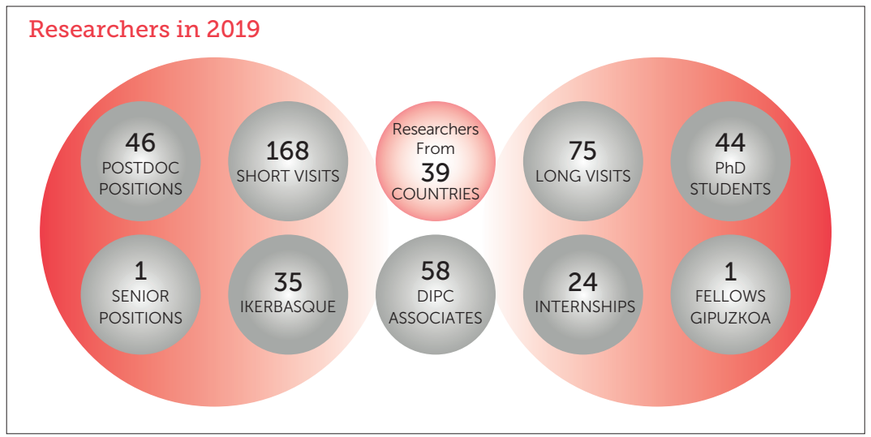
Source Web of Science Core Collection (all years and all indexes, 06/04/2020)



In addition to doing research, DIPC's annual strategic agenda of actions foster exchange with scientists from around the world. Included in the program are Seminars by international experts which cover particular research topics, the DIPC Colloquia which are colloquium-style lectures by outstanding speakers covering all areas of natural sciences, Workshops on specific subjects of interest, and the DIPC Schools and Courses which focus on learning particular skills.

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

The core of the DIPC Community is made up of local scientists as well as PhD students and postdoctoral researchers who come from other institutions to complete their training and hone their expertise with us. DIPC Associates are situated in other centers at different faculties of the University of the Basque Country and at the Materials Physics Center. Our scientists act as hosts for the large number of international visiting researchers and retain the scientific-technical knowledge locally which helps to develop long term DIPC research projects. Among the local host community, there are also Ikerbasque Researchers and Gipuzkoa Fellows.



DIPC Supercomputing Center

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

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

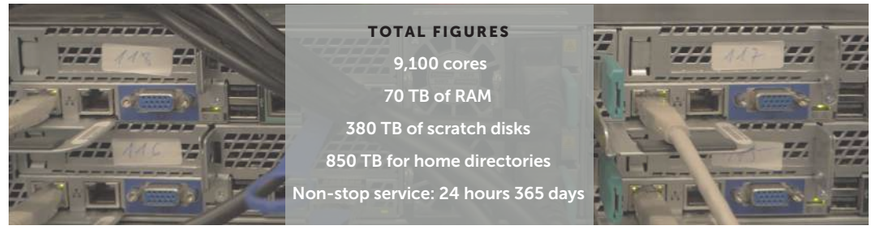
"The variety and power of the computing resources of DIPC, and its constant upgrade, allow the permanent confrontation of a wide range of numerical simulations that put DIPC and other research centers of the Basque Country at the forefront in research"

Txomin Romero Asturiano
Director of the DIPC Supercomputing Center

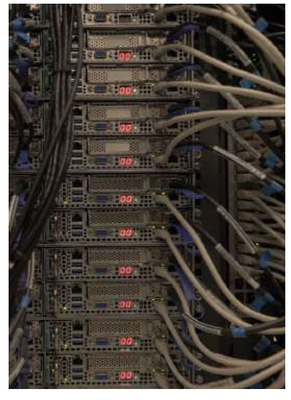
Current computing resources

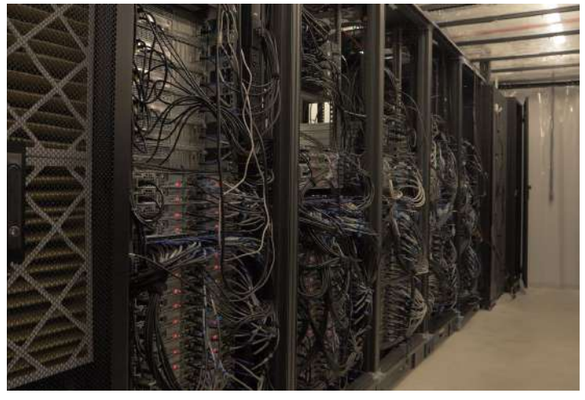
The Center has three rooms to host the HPC systems. These rooms have an isolated electrical connection, communications infrastructure, humidity, electricity consumption and temperature control sensors, various uninterrupted power supply systems, refrigeration systems, automatic fire-extinguishing systems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

As of 2019, the Center has several supercomputers covering a wide range of computational needs. Its main facility is the supercomputer ATLAS, a cluster with Xeon nodes (from 24 cores and 128 GB of RAM small nodes to large shared memory nodes with 52 cores and 1.5 TB of RAM in a single operating system image). With more than 8,000 cores and 70 TB of RAM, ATLAS is one of the more powerful supercomputers in Spain. In addition, some of our supercomputers have NVIDIA Tesla P40 technology for GPGPU programming, Xeon Phi technology and ARM and AMD processors based nodes.



More than 280 researchers from DIPC and other research centers of the Basque Country such as the UPV/EHU, the CSIC-UPV/EHU Materials Physics Center, CIC nanoGUNE, CIC Biomagune, IIS BioDonostia, several BERCs (like BCAM, BCBL or BC3) and Ikerbasque used this computational infrastructure in 2019.





Science Communication

It is our duty to spread scientific culture to society

DIPC has established a solid science communication program becoming a reference for scientific culture both at educational level and for the general public. 2019 was a very special year as the fourth edition of the festival Passion for Knowledge organized by DIPC was celebrated in the Basque Country. Also, in the last years, permanent collaborations with cultural agents such as Kutxa Fundazioa, Elhuyar Foundation, The Chair of Scientific Culture of the University of the Basque Country (UPV/EHU), Jot Down Magazine, the Basque Film Archive or the San Sebastián Film Festival, as well as research institutions such as the Materials Physics Center CFM (CSIC-UPV/EHU) and CIC nanoGUNE have explored new combinations to put science in the spotlight of our cultural life.

95 EVENTS

32,721 ATTENDEES

19 P4K

PASSION FOR KNOWLEDGE

Passion for Knowledge (P4K) festival is a celebration of learning and curiosity involving the active participation of thousands of citizens. The festival's fourth edition was held from 30 September to 5 October 2019 mainly in San Sebastián, with complementary activities also organised in the cities of Bilbao, Pamplona and Bergara.

In 2019, the International Year of the Periodic Table of Chemical Elements was celebrated and P4K festival payed tribute to one of its components: tungsten, also known as wolfram (W), which was isolated in Bergara in 1783 by the Elhuyar brothers.

In addition to the plenary talks, the polyhedral program included activities targeted at different audiences, such as encounters between secondary school students and scientists, Naukas sessions, exhibitions, a special session for children and families, performances and screenings, among others. As a whole, the festival attracted more than 11,800 spectators.

Victoria Eugenia Theatre in San Sebastián, main venue of Passion for Knowledge 2019.

P4K Plenary Lectures featured prestigious researchers behind some of the greatest scientific discoveries of recent years. The open talks held in the Victoria Eugenia Theatre, the Guggenheim Museum and the Baluarte Conference Centre allowed anyone interested in science to continue learning alongside Nobel Laureates and world-class experts.

30 SEPTEMBER – 5 OCTOBER 2019

Plenary Lectures

Dame Jocelyn Bell Burnell Astrophysics, Oxford University, UK
Einstein, Eddington and a solar eclipse

Serge Haroche Physics, Collège de France, France
Nobel Laureate in Physics 2012
Reflections about the scientific truth

Juan Ignacio Cirac Theoretical Physics, Max Planck Institut für Quantenoptik, Garching, Germany
¿Cómo serán los superordenadores del futuro?

Albert Fert Condensed Matter Physics, Université Paris-Saclay, France
Nobel Laureate in Physics 2007
Fundamental physics at the base of the technologies for information age

Barry Barish Physics and Astrophysics, Caltech and UC Riverside, USA
Nobel Laureate in Physics 2017
From Einstein to Gravitational Waves

María Martinón-Torres Paleoanthropology, CENIEH, Spain
Homo sapiens y la sombra del ciprés

Sir John Pendry Photonics, Imperial College London, UK
Capturing light on the nanoscale

Ginés Morata Genetics, Centro de Biología Molecular Severo Ochoa, Spain
La Biología del siglo XXI: la manipulación de información genética y la sociedad del futuro

Nekane Balluerka Behavioural Sciences Methods, (UPV/EHU), Basque Country, Spain
Euskal Herria eta Zientzia: herri txiki baten garapen handia

William Friedman Botany, Harvard University, USA
Who discovered evolution?

Jean-Marie Lehn Supramolecular Chemistry, Université de Strasbourg, Strasbourg, France
Nobel Laureate in Chemistry 1987
Steps Towards Life: Chemistry!

Maria Vallet-Regí Smart Biomaterials, UCM, CIBER-BBN, Spain
Nanoagente de sílice para combatir enfermedades de hueso

Christophe Rossel Physics, IBM Research- Zurich, Switzerland
Is Artificial Intelligence heading towards a technological singularity?

Jean-Pierre Sauvage Chemistry, Université de Strasbourg, France
Nobel Laureate in Chemistry 2016
Molecular Machines in Biology and in Chemistry

Pamela Diggle Botany, University of Connecticut, USA
Plants in our changing world

Dudley Herschbach Chemical Physics, Harvard University, USA
Nobel Laureate in Chemistry 1986
Celebrating Mendeleev

www.p4k.dipc.org

BERTSO PASSION

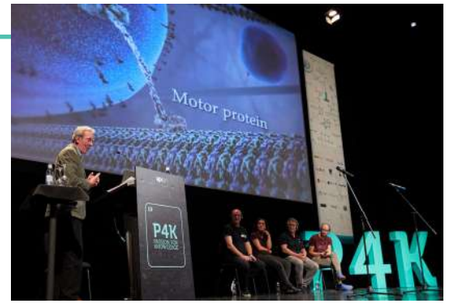
02/10/2019
Victoria Eugenia Theatre,
Donostia/San Sebastián

Passion for Knowledge mixed on stage science and bertsolarism, the art of singing extemporaneously composed songs in Basque. The session featured four scientists involved in important scientific discoveries of recent years, and four bertsolaris, the top representatives of extempore verse singers.

Presenter:
Felix Zubia

Bertsolaris:
Amets Arzallus
Maialen Lujanbio
Andoni Egaña
Iñaki Murua

Scientists:
William Friedman
Dudley Herschbach
María Martinón-Torres
Jean-Pierre Sauvage



IKERBASQUE AWARDS

01/10/2019
Victoria Eugenia Theatre,
Donostia/San Sebastián

Ikerbasque organized the first edition of awards to women researchers and female scientists in 2019. P4K festival featured the award-winning scientists in a special session in which they explained their scientific breakthroughs to the large audience of the festival.

Condensed Matter Physics,
Ikerbasque researcher at DIPC
Maia Garcia Vergniory
Materiales del futuro

Bionanotechnology,
Ikerbasque researcher at CIC biomaGUNE
Aitziber López-Cortajarena
Ingeniería de proteínas:
¿El futuro de nuevas terapias, procesos biotecnológicos y biomateriales?

PASSION TXIKI

05/10/2019
Club Room, Victoria Eugenia Theatre,
Donostia/San Sebastián

This mini science festival targeted at children and their families was mainly held in Basque. During the practical workshop I *Investigate* kids could play and experiment with polymers, light, chemistry and climate change. In the second part, the scientific storyteller Ana Galarraga offered the show *In the laboratory of life* that mixed curious stories and experiments.

CREATIVIUM

23/09/2019–05/10/2019
Carlos Santamaria Center (UPV/EHU),
Donostia/San Sebastián

All creative ideas require a prior process of preparation, during which thoughts mature and take form to culminate in what is known as the moment of enlightenment, or the Eureka! moment. Various researchers have participated in this initiative, which is part of the Mestizajes program. Coordinated by Gustavo Ariel Schwartz with photographs taken by Paula Arbide, Creativium was presented within the festival P4K 2019 and open to the public.

For more information visit:
http://creativium.mestizajes.es

PhD Training

03/10/2019
DIPC Headquarters,
Donostia/San Sebastián

P4K included a dissemination training session addressed at young scientists. A group of PhD students with different backgrounds engaged in a series of activities aimed at enriching their experience and developing their communication skills.

- *Meet the Prof* was an opportunity to discuss on science and its social impact with Nobel Laureate Dudley Herschbach, María Vallet and Sir John Pendry.
- *Dissemination through blogging* was a workshop delivered by Cesar Tomé, editor of Mapping Ignorance, to train writing skills of PhD students.

NAUKAS PASSION

03–05/10/2019
Victoria Eugenia Theatre,
Donostia/San Sebastián

After the keynote talks, some of Naukas best collaborators went up on stage to offer short 10-minute talks to explain science in a fun and original way. Naukas Passion was again organised in collaboration with the Chair of Scientific Culture of the University of the Basque Country (UPV/EHU).

The cherry on the cake of the Naukas Passion section came on the final day of the festival. On Saturday, 5 October, the audience could enjoy with the performance of "'CARBÓN' (COAL), a popular science show written by the neuroscientist and scientific disseminator Xurxo Mariño and the comedian and actor Oswaldo Digón.

top@DIPC Encounters. Zientziarekin solasean!

DIPC organized the 11th edition of the annual Encounters between Nobel Laureates and leading researchers with high schools students with Pedro Miguel Echenique as moderator. Two encounters *top@DIPC* were held in the framework of the festival Passion for Knowledge 2019.

Each encounter featured three internationally renowned researchers from different fields, selected from among P4K 2019 guest speakers. The scientists talked about their passion for science and research and answered the questions asked by students about their lives and experiences throughout the course of their professional careers.

The main aim of these encounters is to foster students' interest in science and technology, and to kindle a passion for knowledge in their young minds.

Telefónica and **EDP naturgas energía**, long time patrons of DIPC, participated and sponsored the Encounters held in Bilbao and San Sebastián respectively, by giving an award to the best question sent by the students. **92 schools** from all over the Basque Country participated in the encounters with an overall participation of **391 students and 98 teachers.**

02/10/2019
Eureka! Zientzia Museoa, Donostia/San Sebastián

Dame Jocelyn Bell Burnell
Oxford University, UK

Jean-Pierre Sauvage
Université de Strasbourg, France
Nobel Laureate in Chemistry 2016

Juan Ignacio Cirac
Max Planck Institut für Quantenoptik,
Garching, Germany

Hosts:
Carlos Tamayo
President of Kutxa Fundazioa
Izaskun Simon
Fundación EDP responsible
Cristina Uriarte
Regional Minister for Education,
Basque Government

04/10/2019
Guggenheim Museum, Bilbao

Albert Fert
Université Paris-Saclay, France
Nobel Laureate in Physics 2007

María Martinón-Torres
CENIEH National Research Center
of Human Evolution, Spain

Christophe Rossel
IBM Research- Zurich, Switzerland

Hosts:
Javier Benito
Director of Telefónica Euskadi
Adolfo Moráis
Deputy Regional Minister for Universities
and Research, Basque Government

Participating students and teachers from around the Basque Country join outside Eureka! Zientzia Museoa in Donostia/San Sebastián at the 11th edition of top@DIPC Encounters

PASSION FOR WOLFRAMIUM

01/10/2019
Seminary of Bergara

Bergara town was designed historic site of science in 2018 due to the discovery of wolframium (W) and other significant breakthroughs that took place in the Royal Seminary during the Enlightenment period. In order to celebrate the International Year of the Periodic Table in 2019, a special event with citizens served to highlight the importance of such discoveries in the presence of the scientists invited to the festival.

Participants: **María Vallet, Dudley Herschbach and Pedro Miguel Echenique**

PASSION FOR KNOWLEDGE COMMITTEE

Chairman of P4K 2019
Pedro Miguel Echenique President of DIPC and Professor at the UPV/EHU

Chairman of P4K 2019
Ricardo Díez Muiño Director of DIPC and scientific CSIC researcher at the Material Physics Centre CFM (CSIC-UPV/EHU)

Executive Committee:

Pamplona's Coordinator
Javier Armentia Director of the Pamplona Planetarium

General Coordinator of P4K 2019
Amaia Arregi Scientific Communication and Dissemination at DIPC

Bergara's Coordinator
Rosa Errazkin Technician at the Laboratorium Museum

PhD training
Paola Ferrario Ikerbasque Researcher at DIPC

Plenary Lectures
Nora Gonzalez Head of Scientific Communication and Dissemination at DIPC

Dynapeutics International Summer School
Xabier López Lecturer and researcher at the University of the Basque Country (UPV/EHU)

Encounters and Passion Txiki
Idoia Mugica Head of Communication at CFM (CSIC-UPV/EHU)

Encounters and Passion Txiki
Itziar Otegui Head of Communication at CIC nanoGUNE

Plenary Lectures
Juan Ignacio Pérez Coordinator of the Chair in Scientific Culture at the UPV/EHU

Dynapeutics International Summer School
Eider San Sebastián Lecturer and researcher at the UPV/EHU

Creativium Exhibition
Gustavo Ariel Schwartz CSIC researcher at the CFM (CSIC-UPV/EHU)

Press Office P4K 2019
Manex Urruzola Head of Elhuyar Communication Unit

For more information visit: p4k.dipc.org

On Zientzia

30/09/2019–5/10/2019
Leidor Theatre, Tolosa,
Victoria Eugenia Theatre, Donostia/San Sebastián

A selection of some of the best videos of On Zientzia, a documentary-type audiovisual project organized by Elhuyar Fundazioa and DIPC which relies on citizen engagement, was screened in different cultural spaces during the festival Passion for Knowledge.

ZIENTZIAKUTXA

Kutxa Fundazioa and DIPC have been organizing a program of dissemination talks aimed at the general public for many years. In 2019, this collaboration materialized in ZientziaKutxa, a monthly program combining local and external speakers, and taking care of the gender balance in the participating researchers as well as variety in the transmission language. Overall, 674 people attended the public lectures within Zientziakutxa.

16/01/2019
Z-Hall, Tabakalera
La biología del siglo XXI. Implicaciones sociales de la manipulación de la información genética
Ginés Morata Centro de Biología Molecular Severo Ochoa (CSIC-AM)

20/02/2019
Kutxa Kluba, Tabakalera
Los datos y la inteligencia artificial en el mundo de hoy
Humberto Bustince Nafarroako Unibersitate Publikoa - Universidad Pública de Navarra

27/03/2019
Kutxa Kluba, Tabakalera
NANOciencia-ficción
Arantzazu García-Lekue Ikerbasque, DIPC

29/04/2019
Kutxa Kluba, Tabakalera
Cultura y evolución humana
Juan Ignacio Pérez UPV/EHU, DIPC

09/05/2019
Ruiz Balerdi Hall, Tabakalera
Women in Science: a historical perspective
Petra Rudolf European Physical Society

22/05/2019
Kutxa Kluba, Tabakalera
Elektroiak iraultza teknologikoaren atarian
Maia García Vergniory Ikerbasque, DIPC

05/06/2019
Ruiz Balerdi Hall, Tabakalera
Ondas gravitacionales: explorando el universo
Alicia Sintes Universidad de les Illes Balears (UIB)

20/07/2019
Eureka! Zientzia Museoa
ZientziaKutxa: historias cósmicas
Simulando la estructura a gran escala del Universo
Raúl Angulo Ikerbasque, DIPC
La búsqueda de los agujeros negros masivos
Silvia Bonoli Ikerbasque, DIPC

CINEMA AND SCIENCE

The second edition of the cinema and science cycle was organized by the Basque Film Archive and DIPC at the Bilbao Fine Arts Museum (Bilbao) and in Tabakalera (Donostia/San Sebastián). Under the name "The Unknown", the program included 12 film projections presented by prestigious scientists, a special event in collaboration with Bang Bang Cinema, together with sessions for scholars and public talks. It is estimated that more than 4,600 people participated in the projections and events.

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

2001: A Space Odyssey (Stanley Kubrick, 1968)
(1) 17/01/2019 (2) 19/01/2019
Physicist **Pedro Miguel Echenique**, UPV/EHU, DIPC

The Incredible Shrinking Man (Jack Arnold, 1957)
(1) 24/01/2019 (2) 26/01/2019
Physicist **Aran Garcia-Lekue**, Ikerbasque, DIPC

Fantastic Voyage (Richard Fleischer, 1966)
(1) 31/01/2019 (2) 02/02/2019
Chemist **Fernando Cossio**, Ikerbasque, UPV/EHU
Physicist **Juan José Sáenz**, Ikerbasque, DIPC

First Man (Damien Chazelle, 2018)
(1) 07/02/2019 (2) 09/02/2019
Physicist **Silvia Bonoli**, Ikerbasque, DIPC

Ex Machina (Alex Garland, 2014)
(1) 14/02/2019 (2) 16/02/2019
Physicist **Juan José Gómez Cadenas**, Ikerbasque, DIPC

The Martian (Ridley Scott, 2015)
(1) 21/02/2019 (2) 23/02/2019
Astrophysicist **Agustín Sánchez-Lavega**, UPV/EHU

A.I. Artificial Intelligence (Steven Spielberg, 2001)
(1) 07/03/2019 (2) 09/03/2019
Physicist **Humberto Bustince**, Universidad Pública de Navarra – Nafarroako Unibertsitate Publikoa

Salyut-7 (Klim Shipenko, 2017)
(1) 14/03/2019 (2) 23/03/2019
Physicist **Maxim Ilin**, CFM (CSIC-UPV/EHU) , DIPC

BANG BANG CINEMA

Blade Runner (Ridley Scott, 1982)
Blade Runner 2049 (Denis Villeneuve, 2017)
(1) 16/03/2019 (2) 02/03/2019
Physicist **Javier Aizpurua**, CFM (CSIC-UPV/EHU)

Hidden Figures (Theodore Melfi, 2016)
(1) 21/03/2019 (2) 30/03/2019
Mathematician **Marta Macho**, UPV/EHU

Annihilation (Alex Garland, 2018)
(1) 23/03/2019 (2) 16/03/2019
Biologist **Ana Zubiaga**, UPV/EHU

Public Lectures

20/02/2019
Bidebarrieta Central Library, Bilbao
Zaude lasai, guztiok gara mosaiko genetikoak eta
Ana Zubiaga biologist at UPV/EHU

06/03/2019
Bidebarrieta Central Library, Bilbao
El Universo en un superordenador
Raúl Angulo physicist at Ikerbasque, DIPC

More lectures were organized in San Sebastián as part of Zientziakutxa cycle and delivered by Ginés Morata, Humberto Bustince and Arantzazu Garcia-Lekue.

Scholar sessions

Special morning sessions for students screened the film "Hidden Figures" (Theodore Melfi, 2016) presented by local researchers and served to reflect on gender equality on science and to revindicate female scientist´s contributions:

19/02/2019 and 26/02/2019
Bilbao
Maia García Vergniory physicist at DIPC
Aitzol García physicist at Ikerbasque, DIPC

13/03/2019 and 20/03/2019
Donostia
Maia García Vergniory physicist at DIPC
Ion Errea physicist at CFM (CSIC-UPV/EHU), DIPC

On Zientzia

13/06/2019

The award ceremony of the 9th. edition of the On Zientzia video contest organized jointly by DIPC and Elhuyar Foundation took place at Kutxa Plaza in Tabakalera. It was later broadcasted at the TV program Teknopolis.

In this edition of On Zientzia, 64 videos participated, among them 31 within the Young Prize category, and 24 videos were in Euskera. The participation was gender balanced for the first time thanks to an active campaign that has increased gradually the amount of female contestants in the last years.

YOUNG PRIZE
CNC fabrikazioa eta gehikuntzazko CNC prozesua
Inge Intxauspe
Asier Cabrejas

BEST VIDEO IN BASQUE
Emergentzia
Ane Aramburu
Unai Razkin

BEST VIDEO
Exoplanetas. Mundos más allá del Sistema Solar
Irene Álvarez
Javier Coronado-Blázquez

SPECIAL MENTIONS
Zu, zientzia
Uxuri Urrate
Glutamato Monosódico
Amyad Raduan

PEOPLE'S CHOICE PRIZE
Ikusmenaren iruzurra
Adrian Martinez
Iñaki Arrieta

For more information visit:
www.onzientzia.tv

SESSIONS FOR KIDS IN THE SAN SEBASTIÁN FILM FESTIVAL

20/09/2019 and 23–27/09/2019
Anoeta Velodrome, Donostia/San Sebastián

In 2019, the San Sebastián Film Festival, DIPC and the Basque Film Archive have collaborated to link two of the city's hallmarks: its dedication to cinema and its high specialization in science. As a result, the film *Tximinoen Erresuma* (Jamel Debbouze, 2015) was scheduled at the Velodrome throughout the week of the San Sebastián Film Festival for students from Gipuzkoa schools. Chosen jointly by the Festival and DIPC, it was projected in a version dubbed into Basque, and presented by DIPC scientists. The latter have precisely been responsible for contextualizing the film and transmitting a positive image of science and its contributions among young attendees. An estimated of 13,000 students from 79 schools have participated in these massive sessions at the Velodrome.

WOMEN IN SCIENCE

11–15/09/2019
Donostia/San Sebastián

DIPC, the Materials Physics Center (CFM CSIC-UPV/EHU), CIC nanoGUNE and CIC biomaGUNE joined together to present a common program on the occasion of the International Day of Women and Girls in Science celebrated internationally the 11th February. More than 50 volunteers from the organizing research centers participated with the goal of conveying a clear message: Science is indeed a girl thing.

11/02/2019 | Koldo Mitxelena Kulturgunea
Hand in Hand public lecture

Reyes Calvo CIC nanoGUNE
Miguel Moreno DIPC, CFM (CSIC–UPV/EHU)

Celia Rogero CFM (CSIC–UPV/EHU)
Sebastian Bergeret DIPC, CFM (CSIC–UPV/EHU)

Aitziber López Cortajarena CIC biomaGUNE
Fernándo López-Gallego CIC biomaGUNE

11/02/2019 | CIC biomaGUNE
12/02/2019 | CIC nanoGUNE
Do you know any female scientist? guided visit for scholar groups

11/02/2019 | DIPC, CFM (CSIC–UPV/EHU)
Meet the scientific world, guided visit for high school students

13/02/2019 | Carlos Santamaria Center
Open Science from the inside out: concept, challenges and implementation seminar for the scientific community

Eva Méndez Universidad Carlos III

14/02/2019 | CFM (CSIC–UPV/EHU)
Amona's power workshop for +55 women

15/02/2019 | CIC nanoGUNE
Science is indeed a girl thing workshop for female teenagers

BERTSOZIENZIA

Bertsozientzia is an initiative that seeks to merge two seemingly distant disciplines such as science and bertsolaritza. In 2019, Bertsozientzia was organized for the second time in Guipuzkoa in collaboration with the Chair of Scientific Culture of the UPV/EHU and local collaborators such as The Zarautz On Association, and Lemniskata Goierriko Zientzia Sare Herrikoia.

Under the name of "Jakinduriek mundue erreko dau" (Knowledge will burn the world) each event brought together three scientists and two bertsolaris and was presented by Basque communicator and humourist **Kike Amonarriz**.

12/04/2019 | BEASAIN
Bertsolaris:
Sustrai Colina
Onintza Enbeita
Speakers:
Miren Karmele Gómez
Josu López-Gazpio
Onintze Salazar

14/05/2019 | ZARAUTZ
Bertsolaris:
Igor Elortza
Alaia Martin
Speakers:
Gorka Azkune
Miren Karmele Gómez
Oscar Gonzalez

22/05/2019 | TOLOSA
Bertsolaris:
Nerea Ibarzabal
Amets Arzallus
Speakers:
Onintze Salazar
Juan Ignacio Pérez
Gorka Azkune
Josu López-Gazpio

HIGH SCHOOL VISITS

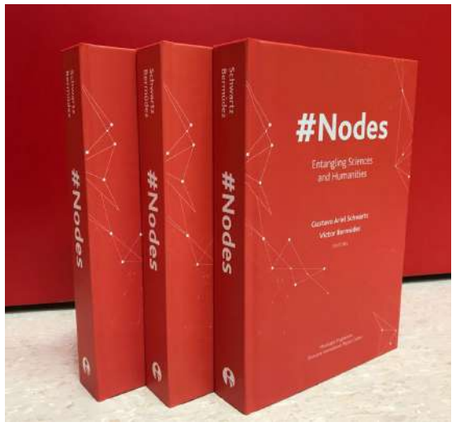
In 2019, DIPC together with the Material Physics Center CFM (CSIC–UPV/EHU) continued the program of visits for groups of high school students launched in 2014. Both centres open their doors so these young students can meet researchers and view their work close up. During 2019 a total of 593 students from 18 schools were hosted.

MESTIZAJES

Mestizajes is a transdisciplinary project aimed at all audiences designed under an innovative and original perspective to foster dialogue between science, literature and humanities. The project is promoted and organized by DIPC within the framework of Euskampus.

Mestizajes proposes different activities such as conferences, seminars, presentations. These activities are done with the collaboration of the San Telmo Museum, Donostia Kultura and the Vice Rectorate of the Guipúzcoa Campus of the University of the Basque Country.

In 2019, the activity mainly focused in the ambitious projects Creativium and #Nodes book.



ENGLISH VERSION OF #NODES

Editorial Intellect Books, Bristol, United Kingdom

#Nodes is a transdisciplinary meeting point in which artists, scientists, writers and humanists from different countries share experiences and reflections about the relevance and possibilities of interactions between different disciplines. This is a book that brings together about 90 contributions around ten thematic areas: Complex networks, Metaphor, Cosmos, Chaos and complexity, Emergence, Perception, Memory, Emotion, Consciousness and Big data. The edition was coordinated by Gustavo Ariel Schwartz and Víctor Bermúdez. Previously in Spanish, in 2019, the book has been published by Intellect Books in English and will be distributed worldwide in collaboration with the University of Chicago Press.

CREATIVIUM

Donostia/San Sebastián

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

The project is based on three pillars: a photobook, a photographic exhibition and a website. The photographic exhibition was inaugurated on the occasion of Passion for Knowledge festival on September 23rd, 2019 in San Sebastián. The book has been published in three languages (Spanish, English and Basque) and the Spanish version has been commercialized through Los Libros de la Catarata.

Creativium has been written and coordinated by Gustavo A. Schwartz, a researcher at the Materials Physics Center (CSIC-UPV / EHU), associated to DIPC and director of the Mestizajes Program. The photographs were taken by Paula Arbide.

27/11/2019
FNAC, Donostia/San Sebastián
Presentation of Creativium
Gustavo Ariel Schwartz and Paula Arbide

VISITING RESEARCHERS
Donostia/San Sebastián

In 2019, two researchers visited DIPC to spend a period of study and research on interdisciplinary subjects within *Mestizajes:*

23–24/9/2019
Creativium Creatividad en la literatura y en la ciencia
Francisco González Fernández Universidad de Oviedo

23–26/9/2019
Analyzing creativity with machine learning and big data
Juan Luis Suárez The CulturePlex Lab, Western University

For more information visit: www.mestizajes.es

SCIENCE WEEK

07–09/11/2019

PhD students, young post-doctoral researchers and communicators from DIPC, Materials Physics Center (CSIC-UPV/EHU) and CIC nanoGUNE participated together with a stand called *Exploring the tiny* world at the Science Week organized by the University of the Basque Country (UPV/EHU) in the Tabakalera - International Centre for Contemporary Culture, Donostia/San Sebastián. School kids, families and citizens could enjoy with hands-on activities and learn about material´s science with more than 30 volunteers from our institutions.

SCIENCE DISSEMINATION CONTEST

Organized annually since 2015 in collaboration with the well-known Spanish cultural magazine Jot Down, the contest recognises the best science dissemination articles. The award ceremony took place within the framework of the Science Jot Down event in Seville with the following winner:

FIRST PRIZE
Murciélagos, buñuelos y el temblor de los indígenas
Pablo Izquierdo

DONOSTIA WEEKINN 2019

DIPC collaborated in the organization of several events within the 6th Innovation Week (Donostia weekINN 2019) organized by Fomento of San Sebastián.

28/10/2019
Baga Biga Faktoria, Donostia/San Sebastián
Zientzia & Fun
Mujeres & Ciencia / Emakumeak & Zientzia
Estefanía Carrasco, María Caffarel, Susana Carregal, Maia García Vergniory and Angela Araujo

29/10/2019
Baga Biga Faktoria, Donostia/San Sebastián
Zientzia & Fun
Fútbol & Ciencia / Futbola & Zientzia
Aitor Bergara and Adrian Odriozola

31/10/2019
Tabakalera, Donostia/San Sebastián
02/11/2019
The Bilbao Fine Arts Museum
Film screening
APPOLLO 11 (Todd Douglas Miller, 2019)
Joxean Fernández, Ricardo Díez Muiño and Euken Sesé

26-31/10/2019
San Martin Market, Donostia/San Sebastián
Exhibition
nanoKOMIK

PRIDE IN SCIENCE

The Materials Physics Center CFM (CSIC–UPV/EHU), CIC nanoGUNE and DIPC joined the international movement Pride in STEM (Science, Technology, Engineering and Mathematics) - which for a few years seeks to give visibility to the LGTBQI collective in science and spread the message that in science diversity is also fundamental.

As part of the first #PrideinSteam initiative in San Sebastián, two lectures of scientific divulgation with LGTBQI perspective and a table/forum for the debate open to all audiences were organized.

05/07/2019
Crypt of Covent Garden, Donostia/San Sebastián
Ciencia LGTBQI, ¿algún problema?
Aitzol García Etxarri
Azul, Rosa u otra cosa
Isabel López Calderón Universidad de Sevilla

Kimikoteka inaugurated the 12th December with a program of activities that extended to 2020.

KIMIKOTEKA

On the occasion of the 150th anniversary of the creation of the periodic table and in parallel with the celebration of the International Year of the Periodic Table in 2019, DIPC conceived KIMIKOTEKA, a project to highlight the importance and beauty of the periodic table.

To this end, a collection of wines build up from the chemical elements of the periodic table served to explain the different chemical, physical and biological processes behind the wine. The chemist Juan José Iruin elaborated a list of 118 wines looking for the major coincidences between the name of the wine and the acronym of the chemical elements. And, to complete that particular collection, DIPC had the collaboration of Rekondo Jatetxea and Goñi Ardoteka, who provided the displayed bottles.

12/12/2019
Koldo Mitxelena lecture hall
Presentation of the KIMIKOTEKA project
Pedro Miguel Echenique Physicist at DIPC and UPV/EHU
Juan J. Iruin Chemist at UPV/EHU

19/12/2019
Koldo Mitxelena lecture hall
The Periodic Table of Wines lecture
Juan J. Iruin Chemist at UPV/EHU

20/12/2019
Goñi Ardoteka
Guided wine tasting
Enrique Osés Sommelier of Goñi Ardoteka
Juan J. Iruin Chemist at UPV/EHU

12/12/2019–19/12/2019
Koldo Mitxelena
20/12/2019–08/01/2020
Goñi Ardoteka
Public exhibition of the KIMIKOTEKA of wines

Scientific Highlights

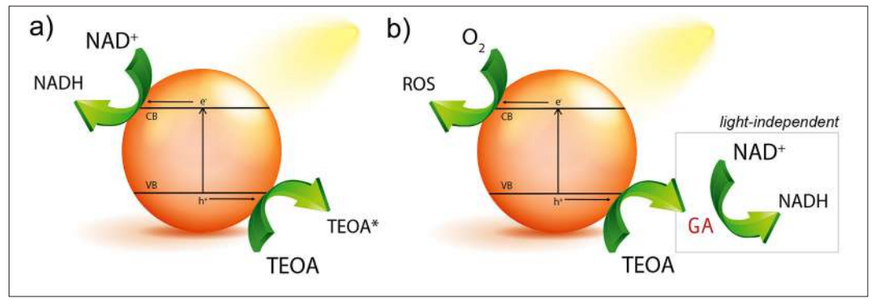
Photocatalytic cofactor regeneration involving triethanolamine revisited: The critical role of glycolaldehyde

Kinastowska K, Liu J, Tobin JM, Rakovich Y, Vilela F, Xu ZT, Bartkowiak W, and Grzelczak M
Applied catalysis B: Environmental 243, 686-692 (2019)

Tapping into the world's largest renewable energy resource is a challenging but essential task due to the increasing appetite for energy from the global society. In contrast to fossil fuels, sunlight distributes evenly over the entire globe, paving the way for it to become a core ingredient of a sustainable society. The need for efficient conversion of light energy into useful fuel pushes academic and industrial communities to find innovative approaches to harvest light and produce solar fuel. Nature solved this issue over two billion years ago through the natural photosynthesis, a process based on water oxidation and simultaneous photoregeneration of biomolecules (cofactors) that later take part in the production of carbohydrates (Calvin cycle). The photoregeneration of cofactor molecules, e.g., NADH, using organic or inorganic photocatalysts is a cost-efficient strategy of producing added-value chemicals since NADH can be implemented in many enzymatic reactions and even recycled.

The difficulty in photoregeneration of cofactor molecule remains in the need of using another molecule —sacrificial electron donor— that donates electron(s) to photoexcited photocatalyst to be later passed to the acceptor (NAD+) (a). Of course, water is the most wanted electron donor (Nature's solution), but it is a very stable molecule, pushing the scientists to find alternative solutions. One of such alternatives is triethanolamine (TEOA) that has become a flagship electron donor in research labs since its first implementation in the late seventies. Although its demonstrated electron-donating character, little is known on the exact degradation pathway, especially in the process of cofactor regeneration.

A team of researchers, including Ikerbasque researchers Yury Rakovich (CFM & DIPC) and Marek Grzelczak (DIPC), shows that triethanolamine can decompose to glycolaldehyde, an intermediated product that is able of reducing NAD+ to NADH, regardless the presence of light (b). These findings show that degradation of triethanolamine and regeneration of cofactors molecules are not necessarily coupled processes when oxygen is present in the mixture, as thought for many years. The pre-irradiation of TEOA solution in the presence of state-of-the-art photocatalysts including conjugated microporous polymer, carbon nitride, platinum nanoparticles and titanium dioxide leads to the formation of a large amount of glycolaldehyde, which induces NADH regeneration in the dark, even after the photocatalyst removal.



Schematic illustration of cofactor photoregeneration mechanism (transfer of two electrons and a proton to NAD^+ to give NADH) in the presence of triethanolamine (TEOA) as an electron donor and semiconductor as a photocatalyst. Semiconductor can be organic or inorganic material. (a) Commonly accepted reaction route postulating simultaneous TEOA oxidation and NAD^+ reduction on the material surface. (b) Proposed alternative reaction pathway involving TEOA oxidation to glycolaldehyde - an intermediate able to reduce NAD^+ even after the removal of both light and photocatalyst. Note the critical role of molecular oxygen in the process, which competes with NAD^+ for receiving an electron.

Oxygen-assisted photodegradation of triethanolamine leads to the formation of glycolaldehyde that is capable of reducing cofactor molecules

Apart from obtaining a better mechanistic picture of cofactor regeneration, these basic-research results came with exciting perspectives for future works. It turns out that glycolaldehyde (the simplest form of sugar) is of high value in the field of prebiotic chemistry. Glycolaldehyde is an essential intermediate in the so-called formose reaction, a process that involves the self-accelerated synthesis of biologically-relevant sugars (e.g. ribose) from formaldehyde as a starting material.

DIPC HIGHLIGHT 2019

Cholesteric aggregation at the quinoidal-to-diradical border enabled stable n-doped conductor

Yuan D, Huang D, Medina S, Carreras A, Zhang C, Zou Y, Jiao X, McNeill CR, Zhu X, Di C, Zhy D, Casanova D, and Casado J
Chem 5, 964-976 (2019)

Doping is a vital strategy in achieving high-performance organic electronic devices. Compared to p-doped materials, there are only a few complementary n-doped conductors reported and all of these are unstable in ambient conditions, a limitation for the consolidation of organic materials in the electronic market. The well-known instability of the electrically active radical anions in the n-doped substrates, becomes one of the most critical challenges to solve.

A diradical is a molecular species having two unpaired electrons, in which at least two different electronic states with different multiplicities, electron-paired (singlet state) or electron-unpaired (triplet state), can be identified. Organic diradicals in which there are rings with alternating single and double bonds (Kekulé-type), are intriguing molecules from several points of view. When they possess incipient-to-medium diradical character, unique electrical, optical, and magnetic properties emerge, motivating organic chemists to create a wide range of diradical compounds.

Now, a team of researchers that includes DIPC researchers Abel Carreras and David Casanova (Ikerbasque) has demonstrated that diradical character is one of the conditions for achieving stable n-type doped conducting materials. A series of thienoquinoidal oligothiophenes from dimer to pentamer and substituted with an odd and even number of pyrrolo-dione groups were prepared and proven to be n-dopable materials showing outstanding ambient stability and excellent electrical and thermoelectric behavior (Figure 1). Going from dimer to pentamer, a progressive change in the diradical character and aggregation mode is observed, with the tetramer showing an optimal diradical character that allows favorable intermolecular contacts, while the presence of the two dione groups promotes a cholesteric-like, perpendicular to the long axes of the molecules, stacking (Figure 2). Both features synergistically contribute to form a material with exceptional ambient stability for an n-doped system exhibiting high electrical conductivities and thermoelectric performance.

These findings offer a new design concept to the organic electronic community for the realization of new and improved applications, such as n-doped conductors and in organic thermoelectrics.

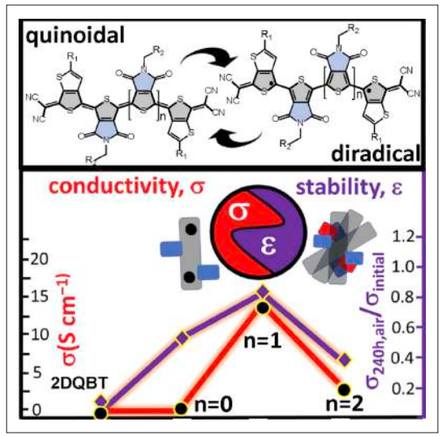


Figure 1. Quinoidal and aromatic resonance structures of the four materials of the family of two-dimensional (2D) quinodimethane oligothiophenes used in this work.

Air-stable n-doped conductors from diradical oligothiophenes

Synergistic action of incipient diradical character and cholesteric-type aggregation

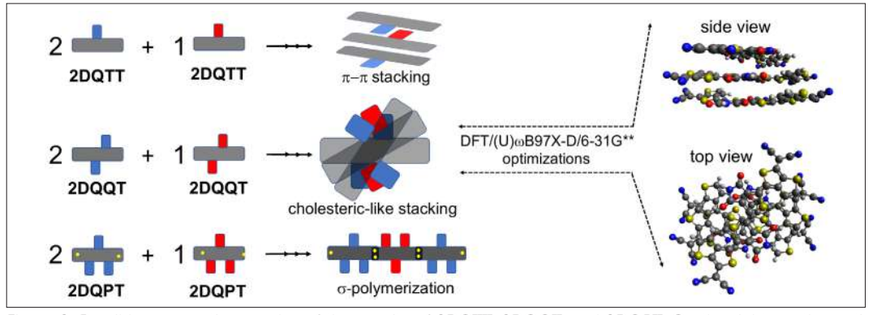


Figure 2. Possible aggregation modes of three units of 2DQTT, 2DQQT, and 2DQPT. On the right are the optimized structures of the cholesteric-like mode of aggregation for neutral and anionic 2DQQT.

Outstanding performance as electrical and thermoelectric materials

DIPC HIGHLIGHT 2019

Theory of spin Hall magnetoresistance from a microscopic perspective

Zhang XP, Bergeret FS, and Golovach VN
Nano Letters 19, 6330-6337 (2019)

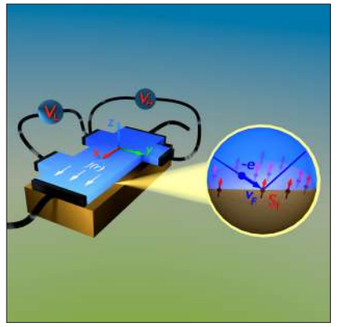
In analogy to the ordinary Hall effect, the spin Hall effect (SHE) describes the spin-dependent deflection of electrons during transport in systems with strong spin-orbit coupling. Such a conversion of charge currents into transverse spin currents is employed now at the forefront of Spintronics to build a new generation of energy-saving electronics, exploiting the spin degree of freedom of the electron.

A manifestation of the SHE in a normal metal (NM) with spin-orbit coupling is the dependence of the magnetoresistance (MR) on the direction of the applied magnetic field when the metal is in contact with a magnetic insulator (MI), such as in NM/MI structures. This effect, called spin Hall magneto-resistance (SMR), has been observed in several experiments as a modulation of the MR signal when the magnetization direction of the MI is changed by an external magnetic field. The origin of SMR lies in the electron's spin-dependent scattering at the NM/MI interface. Thus, by changing the mutual angle between the polarization of spin current and the MI magnetization, one is able to modulate the rate at which the electron spin relaxes.

Although the SMR theory is well established and provides a good qualitative description of the effect, it does not describe the dependence of the resistivity on the strength of the applied magnetic field B, nor on the temperature T. The interface parameters, which are at the heart of the SMR effect, have traditionally been regarded as phenomenological ones in every experiment, because their computation was thought to be a formidable task which could only be carried out by *ab initio* methods.

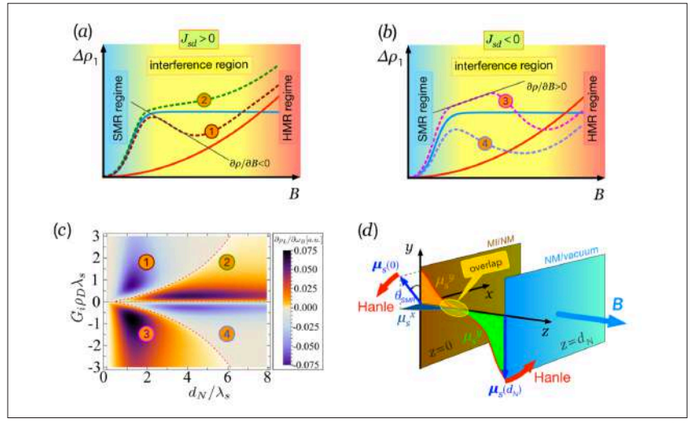
Originally the SMR was observed in Pt thin films deposited on the insulating ferrimagnet $Y_3Fe_5O_{12}$ (YIG). Recent experiments explored other MIs and showed that the SMR effect depends strongly on both B and T, as well as on the magnetic state of the MI. A theory accounting for both the microscopic nature of magnetism in the MI and the spin dynamics of the conduction electrons in the NM near the interface was strongly desired.

In this work, a DIPC team from the Mesoscopic Physics Group presents a general theory of the electronic transport in NM/MI structures. The spin-dependent scattering at the NM/MI interface is described via a microscopic model based on the exchange coupling between local moments on the MI surface and itinerant electrons in the NM. In this theory, the temperature and magnetic-field dependence of the interfacial kinetic coefficients (such as spin-mixing conductance) is expressed in terms of spin–spin correlation functions in the MI.



Sketch of a Hall bar fabricated from a thin metallic film (blue) deposited on the surface of a magnetic insulator (brown). The electron scattering at the interface during which the electron spin interacts with local moments on the surface of the MI is at the heart of the SMR effect.

The theory presented in this work provides a tool to reveal by electric measurements the magnetic properties of interfaces



Different behaviors of the MR predicted by the microscopic theory for a ferromagnetic (a) and antiferromagnetic (b) exchange coupling between the localized moments of the MI and the conduction electrons in the NM. (c) Separation of the parameter space (dN, Gi) into different regimes of interest, with dN being the thin-film thickness and Gi the imaginary part of the spin-mixing conductance. The regions 1–4 correspond to the four kinds of behavior shown in (a) and (b). (d) Sketch of the spin accumulation μs at the thin-film interfaces as created by the SHE and altered by the SMR and HMR effects.

The theory presented in this work does not only explain experiments on a variety of magnetic insulators, such as YIG, EuS, and $LaCoO_3$, but also provides a tool to reveal by MR measurements the magnetic properties of NM/MI interfaces. Furthermore, the theory predicts novel striking behaviors of the MR as a function of B-field, which can be understood in terms of an interplay between the SMR and the Hanle effects.

A complete catalogue of high-quality topological materials

Vergniory MG, Elcoro L, Felser C, Regnault N, Bernevig BA, and Wang ZJ
Nature 566, 480-485 (2019)

Once thought rare, strangely behaving substances called "topological materials" are in fact quite common, a finding that bodes well for their potential to unlock new capabilities for future electronics. An international team of researchers has assembled an online catalog, based on the periodic table, to make it easy to design new versions of these unusual materials. An article accompanying the database was published in the journal Nature on February 28, 2019.

In a major step forward for an area of research that earned the 2016 Nobel Prize in Physics, an international team has found that substances with exotic electronic behaviors called topological materials are in fact quite common, and include everyday elements such as arsenic and gold. The team created an online catalogue (www.topologicalquantumchemistry.com) to make it easy to design new topological materials using elements from the periodic table.

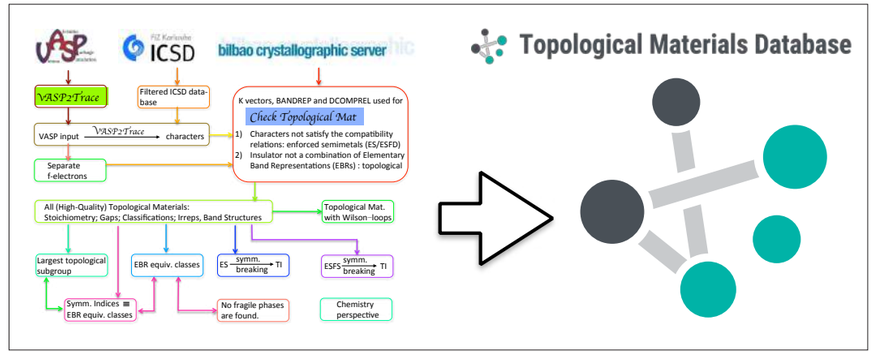
These materials have unexpected and strange properties that have shifted scientists´ understanding of electrons behaviour. Researchers hope these substances could form the basis of technologies of the future, such as low-power devices and quantum computing. For instance, their surfaces can conduct electricity without resistance, so they are potentially faster and more energy-efficient than today´s technologies.

Their name comes from an underlying theory that draws on topology, a branch of mathematics that describes objects by their ability to be stretched or bent.The beginnings of the theoretical understanding of these exotic states of matter formed the basis of the 2016 Nobel Prize in Physics, shared among Princeton University professor F. Duncan Haldane, the Sherman Fairchild University Professor of Physics, and J. Michael Kosterlitz of Brown University, and David J. Thouless, University of Washington, Seattle.

Until recently, only a few hundred of the more than 200,000 known inorganic crystalline materials have been characterize as topological; they were thought as anomalies. However, an international team, including researchers from Princeton; the Donostia International Physics Center in San Sebastián, Spain; the Ikerbasque Basque Foundation for Science; the University of the Basque Country; École Normale Supérieure Paris and the French National Center for Scientific Research; and the Max Planck Institute for Chemical Physics of Solids, found now that topology is ubiquitous at materialsy.

The team investigated about 25,000 inorganic materials whose atomic structures are experimentally known with precision, and classified in the Inorganic Crystal Structure Database. And the results show that rather than being rare, more than 27% of materials in nature are topological.

The researchers made the newly created online database available at www.topologicalquantumchemistry.com. It allows visitors to select elements from the periodic table to create compounds that the user can then explore for its topological properties. More materials are currently being analyzed and placed in a database for a future publication.



The figure shows the different codes and calculations used in our search for topological materials. The open-source code VASP2Trace and end-user button CheckTopologicalMat are available online at www.cryst.ehu.es/cryst/checktopologicalmat, and can check the topology of any material.

Two factors allowed the complex task of topologically classifying the 25,000 compounds.First, two years ago, some of the present authors developed a theory, topological quantum chemistry, published in Nature in 2017, which allowed for the classification of the topological properties of any material from the simple knowledge of the positions and nature of its atoms.Second, in the current study, the team applied this theory to the compounds in the Inorganic Crystal Structure Database. In doing so, the authors needed to devise, write, and modify a large number of computerized instructions to calculate the energies of electrons in the materials.

The authors wrote several sets of codes that obtain and analyze the topology of electrons in real materials. The authors have made these codes available to the public through the Bilbao Crystallographic Server (http://www.cryst.ehu.es/cgi-bin/cryst/programs/topological.pl). With the help of the Max Planck Supercomputer Center in Garching, Germany, the researchers then ran their codes on the 25,000 compounds.

Computationally, it was a very intensive work, but Fortunately, the theory showed that by just looking at what the electron "does" only in part of the parameter space you can obtain the topology of the system. This means that it is necessary to compute only a fraction of the data that was needed previously.

The team is now working to classify the topological nature of the roughly 45,000 compounds in the database that are not part of the "high-quality" database. The next steps involve identifying the compounds with the best versatility, conductivity and other properties, and experimentally verifying their topological nature. The authors of the work said that "One can then dream about a full topological periodic table".

DIPC HIGHLIGHT 2019

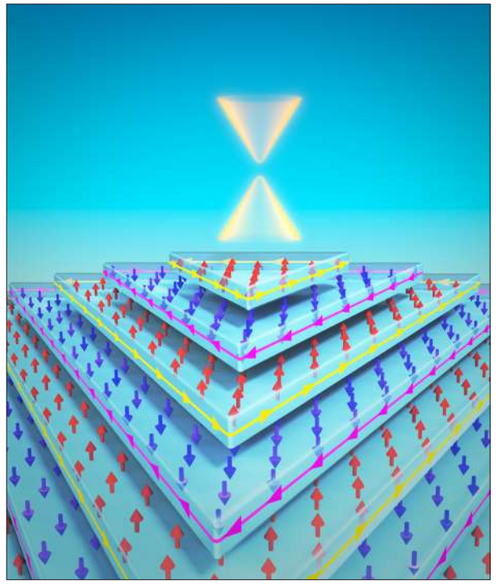
Antiferromagnetic topological insulator $MnBi_2Te_4$

[1] Prediction and observation of an antiferromagnetic topological insulator
Otrokov MM, Klimovskikh II, Bentmann H, Estyunin D, Zeugner A, Aliev ZS, Gaß S, Wolter AUB, Koroleva AV, Shikin AM, Blanco-Rey M, Hoffmann M, Rusinov IP, Vyazovskaya AY, Eremeev SV, Koroteev YM, Kuznetsov VM, Freyse F, Sánchez-Barriga J, Amiraslanov IR, Babanly MB, Mamedov NT, Abdullayev NA, Zverev VN, Alfonsov A, Kataev V, Büchner B, Schwier EF, Kumar S, Kimura A, Petaccia L, Di Santo G, Vidal RC, Schatz S, Kißner K, Ünzelmann M, Min CH, Moser S, Peixoto TRF, Reinert F, Ernst A, Echenique PM, Isaeva A, and Chulkov EV
Nature 576, 416–422 (2019)

[2] Unique Thickness-Dependent Properties of the van der Waals Interlayer Antiferromagnet $MnBi_2Te_4$ Films
Otrokov MM, Rusinov IP, Blanco-Rey M, Hoffmann M, Vyazovskaya AY, Eremeev SV, Ernst A, Echenique PM, Arnau A, and Chulkov EV
Physical Review Letters 122, 107202 (2019)

Ever since the discovery of topologically-nontrivial materials, a magnetically ordered phase in an insulating compound had never been observed to coexist with such a type of electronic order as a topological insulator state. In our recent studies, we report on this kind of electronic behavior in the $MnBi_2Te_4$ compound, which turns out to be an intrinsic antiferromagnetic topological insulator.

Magnetic topological insulators are narrow-gap semiconductor materials that combine non-trivial band topology and magnetic order. Unlike their nonmagnetic counterparts, magnetic topological insulators may have some of the surfaces gapped due to breaking of the time-reversal symmetry, which enables a number of exotic phenomena with potential applications in spintronics. So far, magnetic topological insulators have only been created by means of doping nonmagnetic topological insulators with 3*d* transition metal elements. However, such an approach leads to strongly inhomogeneous magnetic and electronic properties of these materials, restricting the observation of important effects to very low temperatures. Finding an intrinsic magnetic topological insulator, i.e. a stoichiometric well-ordered magnetic compound, could be an ideal solution to these problems, but no such material had been observed to date. In our recent work [1], using density-functional theory, we predict and further confirm by means of structural, transport, magnetic, angle- and spin-resolved photoemission spectroscopy measurements the realization of the antiferromagnetic topological insulator phase, which is hosted by the van der Waals layered compound $MnBi_2Te_4$. An interlayer antiferromagnetic ordering makes $MnBi_2Te_4$ invariant with respect to the combination of the time-reversal (Θ) and primitive-lattice translation ($T_{1/2}$) symmetries, $S = \Theta T_{1/2}$, giving rise to the Z_2 topological classification of antiferromagnetic insulators. We find $Z_2 = 1$ for $MnBi_2Te_4$, which confirms its topologically nontrivial nature. The S-breaking (0001) surface of $MnBi_2Te_4$ exhibits a giant band gap in the topological surface state, as evidenced by *ab initio* calculations and photoemission measurements. These results culminate almost a decade-long search of an antiferromagnetic topological insulator, a possibility of existence of which was predicted in 2010. In a broader sense, $MnBi_2Te_4$ is the first intrinsic magnetic topological insulator realized experimentally.



Artistic representation of the stepped surface of $MnBi_2Te_4$ with the characteristic electronic feature of a magnetic topological insulator (the so-called Dirac Cone) shown above. The red and blue arrows refer to the local magnetic moments of the Mn atoms, which show alternate directions from one terrace to the next, i.e., antiferromagnetic order. The yellow and pink lines, as well as their respective arrows show the directions of propagation of the electric currents at the edges, which are opposite between neighbouring edges (this is known as half-integer quantum Hall effect).

The antiferromagnetic topological insulator $MnBi_2Te_4$ is a unique platform allowing the realization of at least four different quantum Hall effects, some of which have already been observed very recently

The quantum effects featured by $MnBi_2Te_4$ are potentially useful for the development of a new generation magneto-electronic devices

In the two-dimensional limit, $MnBi_2Te_4$ is predicted [2] to show a unique set of thickness-dependent magnetic and topological transitions, which drive it through ferromagnetic and (un)compensated antiferromagnetic phases, as well as quantum anomalous Hall state and its zero plateau. Thus, $MnBi_2Te_4$ is the first stoichiometric material predicted to realize the zero-plateau quantum anomalous Hall state intrinsically. This state was earlier predicted to host the axion insulator phase.

The discovery of the first antiferromagnetic topological insulator opens a new field of magnetic topological insulators that focuses on intrinsically magnetic stoichiometric compounds. As an outcome of this, a number of fundamental phenomena are expected to be eventually observed, such as quantized magnetoelectric coupling and axion electrodynamics. Other exotic phenomena could become accessible at temperatures significantly higher than those achieved to date, like the quantum anomalous Hall effect and chiral Majorana fermions.

DIPC HIGHLIGHT 2019

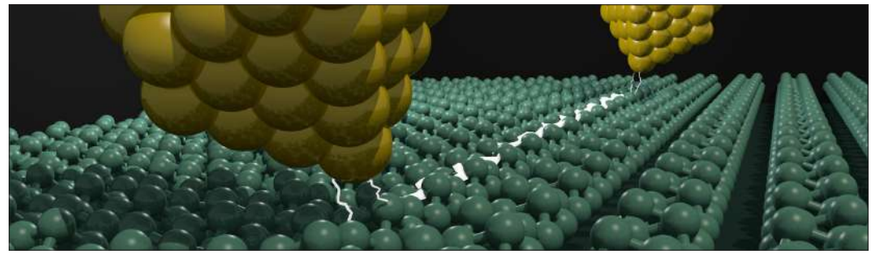
Electronic transport in planar atomic-scale structures measured by two-probe scanning tunneling spectroscopy

Kolmer M, Brandimarte P, Lis J, Zuzak R, Godlewski S, Kawai H, Garcia-Lekue A, Lorente N, Frederiksen T, Joachim C, Sanchez-Portal D, and Szymonski M
Nature Communications 10, 1573 (2019)

Miniaturization of electronic circuits into the single-atom level requires novel approaches to characterize transport properties. Since its invention by Binnig et al. in 1982, the scanning tunneling microscope (STM) is regarded as the method of choice for real-space imaging of the electronic structure of conducting surfaces with picometer resolution. Single-probe STM is also a spectroscopic tool, able to locally probe electronic surface states as a function of the bias voltage in the scanning tunneling spectroscopy (STS) mode. Furthermore, the precision reached in approaching the STM tip apex toward the surface permits for a controlled electronic contact with a single surface atom or molecule.

However, direct determination of the electronic transport properties of a planar atomic-scale wire or circuit lies beyond the single-probe approach. Such characterization requires fabricating metal contacts with high precision, which is usually a challenge. An attractive alternative is the use of multi-probe STM. This method offers high control on the position and geometry of the contacts between the probes and the nanoscale system. But the downscaling of multiprobe instruments toward the atomic level, i.e., where all STM tip apex positions are controlled at the atomic scale, meets many technical obstacles. Although two-probe STM (2P-STM) experiments have been proposed already in the nineties, practical implementations of those propositions were not feasible. The main obstacle was the insufficient stability that caused a lack of both atomic precision in relative probe-to-probe positioning and picometer precision in probe-to-sample contact determination. In fact, only recently 2P-STM experiments have reached the required atomic precision in contacting structures on a surface, however no experimental protocols for extracting transport properties of atomic structures from such experiments had been reported.

An international team of researchers, including members from CFM and DIPC, used for the first time a 2P-STM/STS with probes operating in tunneling conditions over the same atomicscale system to extract detailed information of in-plane electronic transport. They introduced a new method for the determination of the transconductance and demonstrated how it captures energy-resolved information about electronic transport through the unoccupied states from the anisotropic germanium (001) surface. Combining the new experimental protocol with state-of-the-art first-principles calculations they showed that 2P-STS brings information about coherent hot electrons transport in quasi-one-dimensional surface states of germanium (001).



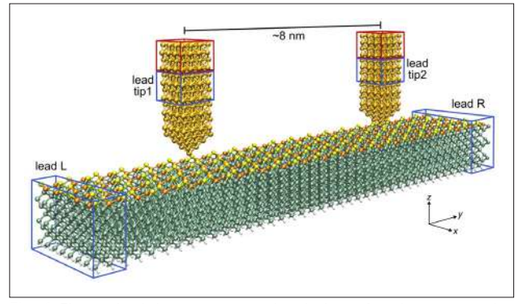


Fig. 1 First-principles transport simulations for the two-probe experiments, represented by a four terminal setup. The electrode regions are highlighted by blue boxes, two of them located at each Ge(001)-c(4×2) slab terminations and the other two at each Au model tip.

The Ge(001) surface consists of buckled Ge dimers forming well-separated parallel rows. The existence of surface dangling bonds introduces additional unoccupied states within the band-gap of the bulk Ge electronic structure. Importantly, weak interactions between adjacent rows result in strong anisotropy of this band structure. Consequently, the reconstructed dimer rows on the bare Ge(001) surface form a series of parallel quasi-1D wires.

In the experiment, electrons injected from one STM tip are collected at a different location at a nanometric distance (down to 30 nm). This was theoretically modeled by a system composed of a twelve-layer Ge(001)-c(4×2) slab contacted by Au tips (Fig. 1). On this self-consistent 4-terminal treatment, two Ge electrodes were connected at each slab termination and other two at the Au model tips. A remarkable agreement was found between the calculated transmission function and the experimental transconductance spectra. The sequential opening of two transport channels within the quasi-one-dimensional Ge dimer rows in the surface gives rise to two distinct resonances in the transconductance spectroscopic signal. These breakthrough simulations also elucidated the transport directionality of the injected hot electrons, revealing a transition from 2D to quasi-1D coherent transport regime.

This work demonstrates that complex experiment setups combined with advanced calculations can provide new insights into transport properties at the nanoscale. The presented techniques are promising and applicable to characterize the quantum transport in 2D materials in general (graphene and beyond). In contrast to standard metal contacts, e.g., fabricated by lithographic techniques, the use of 2P-STM enables a precise adjustment of individual atomic contacts and their resistances, allowing to access the system's intrinsic transport properties, disentangling them from those of the contacts and leads.

DIPC HIGHLIGHT 2019

Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides

Barja S, Refaely-Abramson S, Schuler B, Qiu DY, Pulkin A, Wickenburg S, Ryu H, Ugeda MM, Kastl C, Chen C, Hwang C, Schwartzberg A, Aloni S, Mo SK, Ogletree DF, Crommie MF, Yazyev OV, Louie SG, Neaton JB, and Weber-Bargioni A
Nature Communications 10, 3382 (2019)

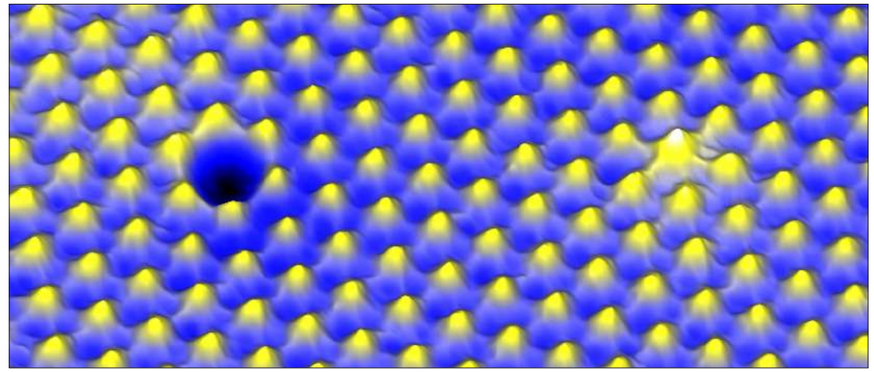
Atomically thin, two dimensional (2D) semiconductors known as transition metal dichalcogenides (TMDs) are not perfect, but their imperfections can actually be a good thing.

Crystal defects are known to modify semiconductor functionality and are expected to have particularly strong impact on the properties of 2D materials, where screening is reduced compared to bulk systems. In particular, 2D-TMDs can feature a variety of different defect geometries and related electronic states. Understanding how defects are structured at the atomic scale, how they are created, and how they interact with electrons are the first steps to designing new advanced materials. However, the experimental identification of individual defects and the direct correlation of these measurements to their electronic structure is far from simple.

In the world of materials science, many researchers assumed that the most abundant defects in TMDs were the result of missing atoms or "vacancies" of sulfur in tungsten disulfide (WS_2), or selenium vacancies in molybdenum diselenide ($MoSe_2$). These missing S or Se atoms are predicted by theory to locally alter the electronic structure of the semiconductor by introducing deep in-gap states (IGS). Consequently, important features in the experimental transport characteristic, optical response and catalytic activity of 2D-TMDs have typically been attributed to chalcogen vacancies, based on indirect support from images acquired by transmission electron microscopy (TEM) and scanning tunneling microscopy (STM). Still, there are a variety of technical challenges that limit the direct correlation of the former atomic scale studies on TMD materials with their macroscopic response, leading to a non-consistent interpretation of the defect type across the current literature.

But as reported in Nature Communications, the defects previously observed with other methods were actually created by oxygen atoms replacing sulfur or selenium atoms, instead of pristine chalcogen vacancies. Oxygen, like sulfur and selenium, is part of the oxygen or "chalcogen" family of elements. And since chalcogens share similar properties, there isn't much change in electronic states of the semiconductor with such replacement: oxygen substituted in the chalcogen sublattice does not form deep in-gap states. Key to this finding was the use of a non-contact atomic force microscope (nc-AFM), with a single carbon monoxide (CO) molecule acting as an ultrasharp "tip" or probe, combined with a scanning tunneling microscope (STM). When used with AFM, the CO-tip images the surface atoms at a very high resolution inaccessible with conventional techniques, which helps to identify the defect's atomic site. Direct correlation to the defect's unique electronic fingerprint was achieved by parallel scanning tunneling microscopy and spectroscopy measurements on the very same defect. These experimental efforts, together with parallel state-of-the-art first-principles ground- and excited-state calculations using density functional theory (DFT) and many-body perturbation theory within the GW approach, respectively, had enabled an unprecedented interrogation of the system.

The comprehensive joint experimental and theorical study provides critical insight for future defect engineering in these systems



Atomic force microscopy image (temperature 4K) of two oxygen atoms replacing selenium atoms in molybdenum disulfide. The oxygen in the left defect replaces a selenium atom in the upper selenium layer, facing the "tip", and appears as a depression in the lattice. The oxygen in the right defect replaces a selenium atom in the bottom selenium layer, opposite the "tip", and slightly pushes the selenium atom upward relative to the pristine lattice.

Direct correlation between the atomic and electronic structures of individual defects in 2D-TMDs is required to achieve a fundamental understanding of the effect of defects on the electronic structure of the material. This work directly relates atomic and electronic structure through combined nc-AFM and STS measurements of individual point defects in monolayer $MoSe_2$ grown by molecular beam epitaxy and in monolayer WS_2 grown by chemical vapor deposition. Although nc-AFM and STM images of chalcogen defects appear to be consistent with vacancies, a comparison with DFT and GW calculations establishes these defects as substitutional oxygen at chalcogen sites, consistent with the lack of IGS in the band structure. Therefore, the comprehensive joint experimental and theoretical study reveals substitutional oxygen as a prolific point defect in 2D-TMDs and provides critical insight for future defect engineering in these systems.

Robust zero-energy modes in an electronic higher-order topological insulator

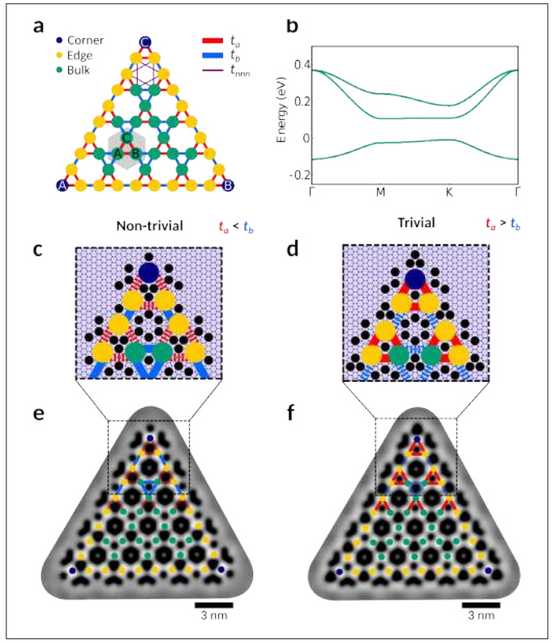
Kempkes SN, Slot MR, van den Broeke JJ, Capiod P, Benalcazar WA, Vanmaekelbergh D, Bercioux D, Swart I, and Smith CM
Nature Materials 18, 1292-1297 (2019)

Quantum simulators are systems that can be engineered and manipulated at will; those are useful platforms for verifying model Hamiltonians and understanding more complex or elusive quantum systems. Different types of platforms have been developed so far, the most prominent and more versatile are based in cold atoms trapped in optical lattices, followed by photonic systems. However, in the past few years, there has been a growing activity about the possibility of engineer quantum simulator with quasi-free electrons confined in artificial lattices. A few years ago, the first artificial electronic lattice was built by positioning carbon monoxide (CO) molecules on a Cu(111) surface, confining the surface-state electrons to a honeycomb lattice. This was followed by other electronic and spin lattices constructed by atomic manipulation via a scanning tunnelling microscope (STM), such as atomic spin chains, the Lieb lattice with *s* orbitals and *p* orbitals, the quasicrystalline Penrose tiling and the Sierpiński gasket with a fractional dimension.

In addition to manipulating the geometry and the dimensionality, it is desirable to engineer and control topological properties in electronic systems. Topological insulators, superconductors and semimetals have attracted enormous attention in recent decades, and their potential use in quantum computers has caused a frantic interest in these systems.

Topological insulators are materials with special universal properties, which are protected against perturbations. Such properties are theoretically described by topology, a branch of mathematics concerned with the properties of geometrical objects that are unchanged by continuous deformations. Concretely, topological insulators are electronic materials that have a bulk band gap like an ordinary insulator but have conducting states on their boundaries, i.e., edges or surfaces. The conducting surface is not what makes topological insulators unique, but the fact that this surface state is particularly robust, potentially due to some symmetry like time-reversal.

We can say, in general, that a topological insulator of *d* dimensions with a given symmetry is insulating in the bulk but supports gapless boundary excitations that cannot be removed by local boundary perturbations without breaking the symmetry. Benalcazar *et al*. published in *Science* a generalization of this bulk-boundary correspondence. In two- and three- dimensions, these insulators exhibit no edge or surface states, respectively, but feature gapless, topological corner excitations corresponding to quantized higher electric multipole moments. These are the so-called higher-order topological insulators (HOTIs), in which the topological states emerge in at least two dimensions lower than the bulk.



Design of the breathing kagome lattice. a) Schematic representation of the finite-size breathing kagome lattice, consisting of three sublattices A, B and C. The unit cell is indicated by a grey hexagon. b) Band structure for the bulk of the lattice shown in (a), calculated using a tight-binding model. c,d) Configuration of CO molecules (black) on a Cu(111) surface (grey background) to establish artificial lattice sites (blue, yellow and green) in a non-trivial (c) and trivial (d) breathing kagome geometry, respectively. Smaller (larger) hopping is indicated by dashed (solid) lines. e,f) Constant-current STM images of the realized non-trivial (e) and trivial (f) kagome lattices.

HOTIs have been experimentally realized in photonic, phononic, topolectrical circuit, microwave circuit and acoustic systems. In this work, we have proposed the first experimental realization of an electronic HOTI.

The researchers create the breathing kagome lattice by manipulating carbon monoxide molecules on a Cu(111) surface using a STM. They engineer alternating weak and strong bonds – this is the breathing – to show that a topological state emerges at the corner of the non-trivial configuration, but is absent in the trivial one.

Different from conventional topological insulators, the topological state has two dimensions less than the bulk, denoting a HOTI. Protected zero modes arise at the corners of the lattice, thus realizing a HOTI with extreme robustness due to the tripartite character of the generalized chiral symmetry. By introducing different types of defects into the lattice, zero modes can be manipulated at will, and the system can be tuned to have an even or odd number of corner modes.

The large degree of control over artificial lattices provides unique opportunities to study electronic topological phases. This new technique allows, in principle, the investigation of any breathing 2D lattice.

These electronic systems are thus complementary to photonic systems, which are designed on a much larger scale, and to the cold-atom set-ups, which offer great control but require nanokelvin temperatures for their operation. The progress in the realization of artificial electronic structures takes a step forward with the inclusion of topology among the parameters to be manipulated.

Extreme decoherence and quantum chaos

Xu ZY, Garcia-Pintos LP, Chenu A, and del Campo A
Physical Review Letters 122, 014103 (2019)

In physics there are some well-known fictional characters: the experimenters Alice & Bob, Maxwell's and Laplace's demons, or some astronauts travelling at incredible speeds, to name a few. But the queen of them all is a cat. Yes, you guess right, that is Schrödinger's cat.

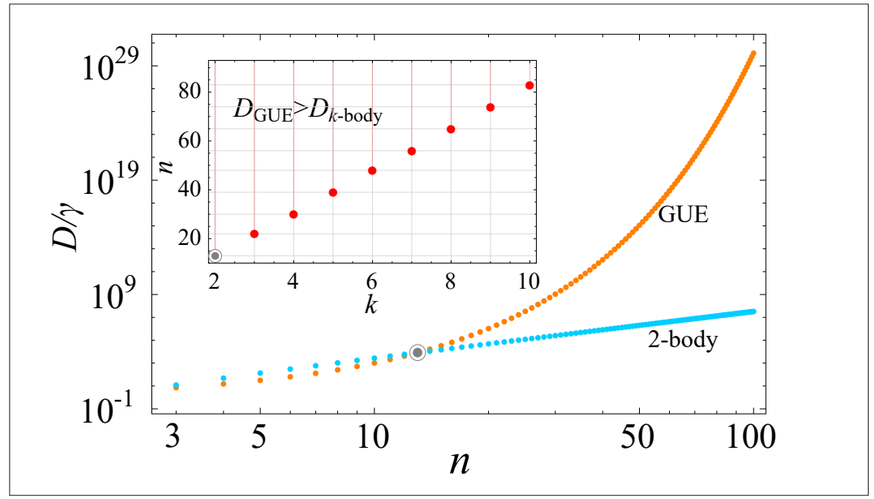
This cat first appeared in a thought experiment designed by Erwin Schrödinger in 1935 with the aim of proving quantum mechanics absurd. The experiment illustrates the paradox regarding the probability of finding, say, a subatomic particle at a specific point of space. According to Niels Bohr's interpretation of quantum mechanics, the position of such a particle remains indeterminate until it has been observed. Schrödinger postulated a sealed vessel containing a live cat and a device triggered by a quantum event, such as the radioactive decay of a nucleus. If the quantum event occurs, cyanide is released and the cat dies; if the event does not occur the cat lives. Schrödinger argued that Bohr's interpretation of events in quantum mechanics means that the cat could only be said to be alive or dead when the vessel has been opened and the situation inside it had been observed. Schrödinger's point was to connect up the oddness of the micro-level to macro-level events.

But, is it really a paradox? Let's assume that what counts as a quantum entity is any object of any size, like a cat. Then any object could be in a superposition of states, as Schrödinger says and finds absurd. And that would be correct, unless we take a broad view of what counts as a measurement. So, although almost any object can in principle exist in a superposition of states, measurements generally suffice to collapse such superpositions well before we or any other creatures could experience them. Thus, the photon detector used to measure the radioactive decay, the cat herself and so on count as quantum entities that could in principle exist in a superposition of states. However the photon detector suffices to collapse the wave function well before a superposition of cat-alive / cat-dead states could occur. This is what is called decoherence.

In general, decoherence is any process in which a quantum mechanical state of a system is altered by the interaction between the system and its environment. It follows that decoherence must be a ubiquitous phenomenon in nature, responsible for the emergence of classical behaviour from the quantum substrate. Thanks to decoherence Schrödinger's cat is a paradox no more.

But the implications of the concept of decoherence are much deeper. For example, decoherence is most commonly attributed to the interaction between the system and something *external* to the quantum system, its *surrounding* environment. However, it can also arise from something *internal*, like the presence of random fluctuations in the system evolution. These can have an *intrinsic* quantum origin, as in the case of continuously monitored systems, or be associated with classical sources of noise.

Noise. If we follow the logic, we will find that the dynamics in each case becomes stochastic, and upon averaging over realizations of the noise processes, decoherence manifests itself in an ensemble perspective, the same concept of ensemble proposed by Josiah Willard Gibbs to talk about the statistical mechanics of thermodynamic systems. Hence, in general, decoherence increases with the system size. This means a real challenge the realizations of quantum information and simulation tasks with complex quantum systems involving a large number of particles and degrees of freedom.



The decoherence rate in chaotic systems described by random matrices (e.g., GUE) is extreme and grows exponentially with the system size. By contrast, for Hamiltonians with local interactions (e.g., 2-body) the growth is simply polynomial.

What if the quantum system is so complex that it is chaotic? In this case decoherence can be expected to be singular due to the enhanced sensitivity to initial conditions.

Understanding the interplay between quantum chaos and decoherence is a long-standing problem. Earlier studies of this subject are mainly focused on the effect of dissipation and decoherence on level statistics, and how to incorporate such effects into the study of quantum systems that are chaotic in the classical limit. Now, a team of researchers, including Ikerbasque Research Professor Adolfo del Campo and Research Fellow Aurélia Chenu (DIPC), poses the question as to what is the ultimate limit to the rate of decoherence of complex quantum systems. This issue is not only of relevance to fundamental and applied aspects of quantum science and technology, but has implications that extend to other fields, including black-hole physics.

In order to find an answer, the researchers introduce a decoherence rate that applies to arbitrary random processes in which the rate of change of a time-dependent quantity depends on the instantaneous value of the quantity but not on its previous history, the so-called Markoffian processes.

Chaotic quantum systems can be described using random matrix theory, originally introduced by Eugene Wigner to deal with the statistics of the spectra of heavy atomic nuclei. Using this theory and the decoherence rate, the researchers show that the dynamics of fluctuating chaotic quantum systems is extreme, in that its rate scales exponentially with the number of particles n. Such scaling has no match in non-chaotic physical systems, where the decoherence rate scales polynomially with n.

These findings suggest that chaotic quantum systems provide an ideal test bed to explore deviations from quantum mechanics, such as those predicted by spontaneous wave function collapse models.

Ultrafast transient dynamics of adsorbates on surfaces deciphered: the case of CO on Cu(100)

Novko D, Tremblay JC, Alducin M, and Juaristi JI
Physical Review Letters 122, 016806 (2019)

Time-resolved pump-probe sum-frequency generation spectroscopy is among the techniques being widely employed in our ambition to monitor and understand elementary reactions of adsorbates on metal surfaces. In these experiments, an intense femtosecond laser pulse (the pump) usually initiates the energy exchange mechanisms between the laser-excited surface electrons and the vibrational modes of both the adsorbates and the surface lattice. Additional time-delayed pulse or pulses (the probe) permit to monitor the ultrafast dynamics followed by the adsorbates.

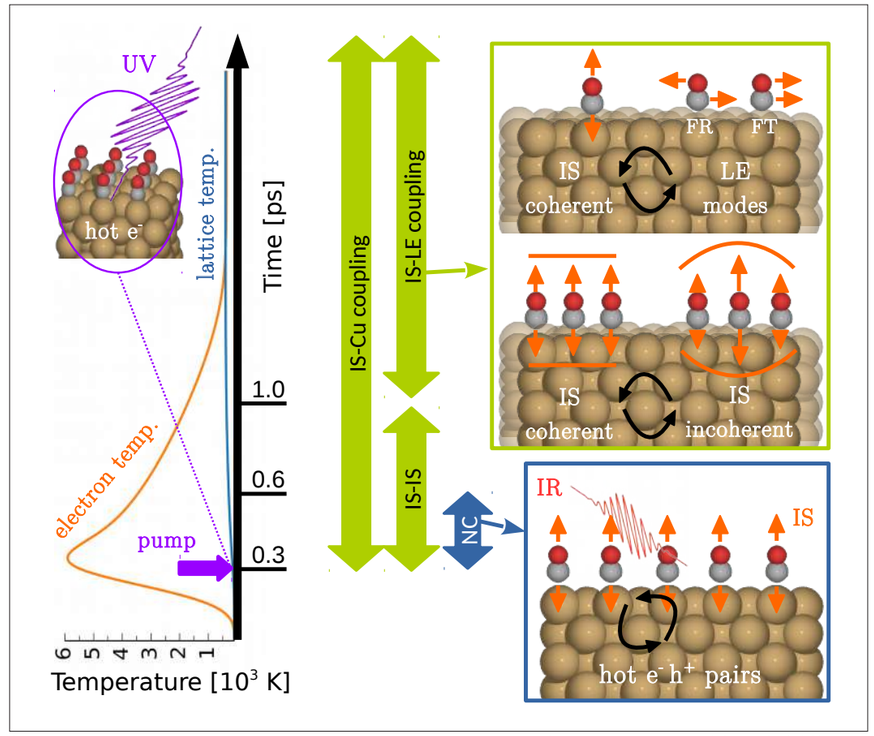
The characteristic transient frequency shift of the active vibrational modes is the property that serves to track how the laser-induced hot-carriers initiate a specific adsorbate reaction, including vibrations, diffusion, and desorption. Unfortunately, the absence of a reliable theoretical framework able to describe this kind of experiment makes difficult to reach a consensus on whether to ascribe these transient shifts to the interaction with low-energy molecular and surface modes or to nonthermal charge transfer between surface and molecular antibonding states. At the end, this uncertainty in determining the nature of the mechanisms kicking the adsorbates out of equilibrium –i.e., electronic, phononic, or both– has been limiting in practice our understanding of ultrafast surface reactions.

Aimed to fill this gap, Novko *et al*. develop in this letter a general first-principles theoretical framework that makes possible to calculate directly the vibrational spectra changes and identify the specific mechanisms behind them. The new theory relies on a recently developed approach based on many-body and density functional perturbation theories that the team extends now to treat nonequilibrium conditions. The first-principles formalism accounts for electron-phonon coupling processes up to second order, including electron-hole pair excitations (the first-order non-adiabatic coupling) as well as vibrational intermode coupling due to the indirect interaction with hot electrons.

As a proof of concept, Novko *et al*. apply this theoretical framework to investigate the early stage dynamics of the benchmark system for electron-induced dynamics at surfaces, non-thermal CO adsorbates (i.e., a molecular overlayer) on Cu(100). This system has recently been monitored with time-resolved sum-frequency generation spectroscopy with unprecedented subpicosecond resolution. It is the new quantitative and predictive theoretical method which finally unveils the microscopic processes behind the reported non-thermal frequency shifts and the accompanying linewidth changes. It also establishes the specific sequence and strength of the non-adiabatic and intermode coupling mechanisms involved.

The researchers find that, contrary to common understanding, the CO internal stretch mode undergoes different mode coupling mechanisms on the subpicosecond and the picosecond timescales. It turns out that the C-O interaction, which is in the end responsible for the IS frequency, is more sensitive to the transient excitations created in the electronic system, while it is the coupling to the excited phonon modes that contributes more to the IS linewidth.

The new theoretical method reveals that different microscopic processes cause the frequency shifts and linewidth changes of the internal stretch mode of CO on metal surfaces.



Schematic chronograph of the coupling mechanisms underlying the IS frequency shifts of CO on Cu(100).

This new theory is destined to be the theoretical counterpart in future vibrational spectroscopy investigations. The time-resolved nanoscopic insights that this theory can provide would be, not only fundamental to the development of vibrational spectroscopy at surfaces, but the reference to advance in our goal of controlling surface reactions at the molecular level.

DIPC HIGHLIGHT 2019

Phonon collapse and second-order phase transition in thermoelectric SnSe

Aseginolaza U, Bianco R, Monacelli L, Paulatto L, Calandra M, Mauri F, Bergara A, and Errea I
Physical Review Letters 122, 075901 (2019)

Thermoelectricity is an interesting material property that allows to transform waste heat into electricity. Good thermoelectric materials need to be good electric conductors and good thermal insulators at the same time, the so called phonon glass and electron crystal. Due to the potential industrial applications of thermoelectric devices a huge research effort is devoted to enhance the thermoelectric efficiency. The intrinsic single crystal of SnSe was recently found to be the most efficient thermoelectric material. In this work we show that very strong anharmonic effects provide its low thermal conductivity, explaining its interesting thermoelectric properties. We expect similar strong anharmonic effects in other good thermoelectric materials.

At room temperature SnSe is a narrow gap semiconductor and at ~800 K suffers a structural phase transition to a phase with higher symmetry. In the high symmetry phase the electronic band gap is decreased while the thermal conductivity is kept very low, properties that provide a very high thermoelectric efficiency. Experimentally, there is discrepancy on the order of the transition, some works claim it is a first order transition and others that it is second order. There is also an experimental discrepancy about the thermal conductivity in the whole temperature range. As it is expected for an orthorhombic system, experiments by Ibrahim et al. show a very anisotropic thermal conductivity, with a value of ~1 W/mK (at 700 K) for the measurements in the YZ plane. Experiments by Zhao et al. show almost no anisotropy and very low values for the thermal conductivity (~0.3 W/mK at 800 K).

In this work, by applying the Landau Theory of Second Order Phase Transitions and the Stochastic Self-Consistent Harmonic Approximation (SSCHA) to calculate the free energy, we show that the transition is second order and it is driven by the collapse of a zone border phonon mode. By making anharmonic phonon calculations within the SSCHA we show that SnSe is a strongly anharmonic material because its phonon spectrum suffers a big anharmonic correction. On top of that, we calculate the phonon spectral functions and strongly anharmonic features are present like shoulders, broad peaks and satellite peaks deviating from the typical harmonic behavior. All these calculations will be very important to understand future inelastic scattering experiments in the high symmetry phase and other materials with second-order phase transitions.

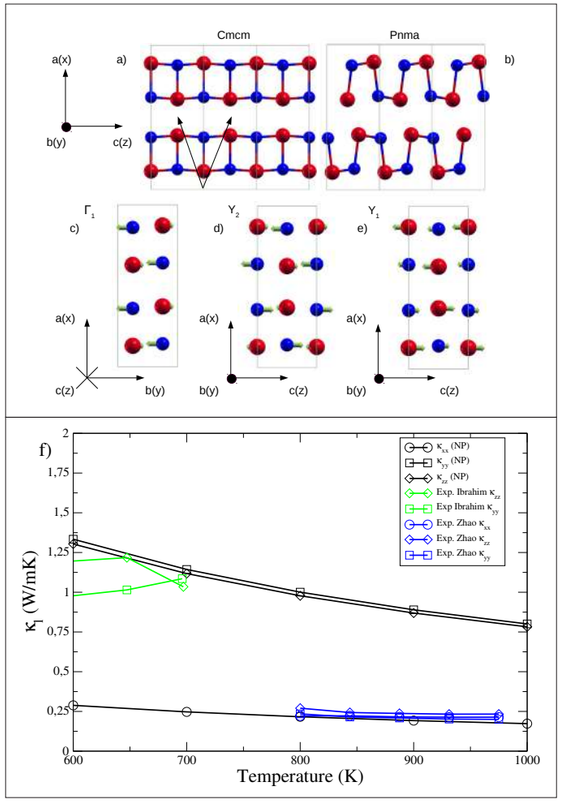


Figure (a) and (b) show the XZ face of the high (Cmcm) and low (Pnma) symmetry phases respectively. Figure (e) shows the atomic displacements of the phonon mode that drives the transition between the two phases. Figure (c) and (d) show atomic displacements that are strongly anharmonic and show non-Lorentzian profiles in the phonon spectral function. Figure (f) shows the experimental and calculated lattice thermal conductivities. The green and blue lines correspond to experiments by Ibrahim et al. and Zhao et al. respectively. Black lines correspond to thermal conductivity calculations including anharmonicity at a non-perturbative level with SSCHA.

The published results unveil the nature of the record thermoelectric tin selenide

Our thermal conductivity calculations in the high symmetry phase clearly show that there is anisotropy between in-plane and out-of-plane measurements and quantitatively agree with experiments by Ibrahim et al.. Therefore, we suggest that the results by Zhao et al. may suffer from non-intrinsic effects. We also show for the first time that non-perturbative anharmonicity is very important to get a thermal conductivity in agreement with experiments.

DIPC HIGHLIGHT 2019

Light induced inverse-square law interactions between nanoparticles: “Mock Gravity” at the nanoscale

Luis-Hita J, Marqués MI, Delgado-Buscalioni R, de Sousa N, Froufe-Pérez LS, Scheffold F, and Sáenz JJ
Physical Review Letters 123, 143201 (2019)

Any physical law in which the magnitude of a physical quantity is proportional to the reciprocal of the square of the distance ($1/r^2$) from the source of that property is known as an inverse-square law. Newton’s law of gravitation and Coulomb’s law are both examples.

When Newton proposed his law of gravitation he was repeatedly asked about the origin of that spooky (as Einstein famously described it) action at a distance. The remarkable Fatio de Duillier–LeSage corpuscular theory, introduced as early as 1690, proposed a mechanical explanation for Newton’s gravitational force in terms of streams of tiny unseen particles (which Le Sage called *ultra-mundane corpuscles*) impacting all material objects from all directions. According to this model, any two material bodies partially shield each other from the impinging corpuscles, resulting in a net imbalance in the pressure exerted by the impact of corpuscles on the bodies, tending to drive the bodies together.

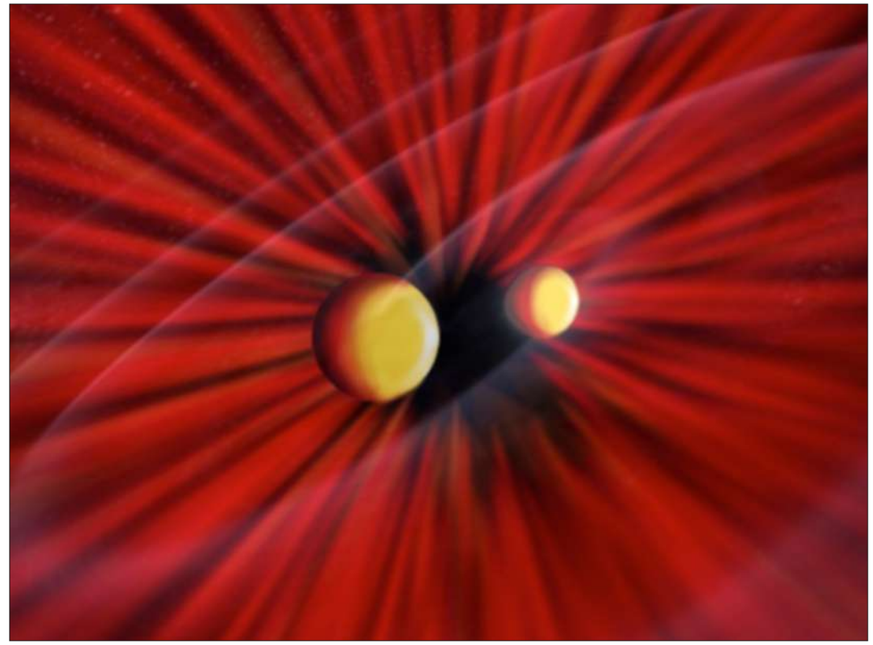
Juan José Sáenz
8/10/1960–22/3/2020

Juan José Sáenz, ‘Mole’ for his many friends and colleagues, was a passionate and generous scientist, known worldwide for his contributions in the field of nano-optics. Mole was a deeply admired, respected and loved member of our community, a kind and joyful man whose memory will stay with us forever.

Agur eta ohore, lagun!

This theory was generalized to electromagnetic waves by Lorentz (1927) who proposed that, due to their mutual shadowing, two absorbing particles in an isotropic radiation field experience an attractive force that follows a gravity-like inverse square distance law. Similar interactions were later introduced by Spitzer (1941) and Gamow (1949), who called it “mock gravity”, in the context of galaxy formation, but their actual relevance in cosmology has never been unambiguously established.

Recent results have demonstrated that the interaction force between non-absorbing dielectric particles and atoms in a quasi-monochromatic isotropic random light field always presents an oscillatory behavior for distances larger than the light wavelength. Now a team of researchers led by Prof. Sáenz at DIPC, show that, under specific resonant conditions, these forces become non-oscillating, $1/r^2$, attractive forces. In other words, at the resonant condition, the interaction forces follow a long-range mock gravity law. This is in strong contrast with the familiar, short range, van der Waals–London and Casimir forces between neutral molecules and particles.



Two particles with resonant absorption under a stochastic field attract each other following a long range gravity-like interaction.

> Light induced interaction forces between identical molecules or plasmonic nanoparticles, whose extinction cross section is dominated by absorption, can follow a true attractive inverse square law

For small separation distances, gravity-like interactions were first predicted by quantum electrodynamics calculations for atoms and molecules and later by a classical approach on Rayleigh nanoparticles leading to analogous results. In these studies, the imaginary part of the polarizability was either not included in the calculations or was taken into account but considered negligible; i.e., radiation pressure effects were neglected. However, as the DIPC team and coworkers show now, these effects dominate the near-field interactions of non-absorbing particles, leading to a different interaction law.

The authors analyzed the interaction forces between identical resonant nanoparticles, in free space or homogeneous media, illuminated by a quasi-monochromatic isotropic random light field. They found that, in contrast with atoms or dielectric particles, the interaction force between plasmonic nanoparticles, whose extinction cross section is dominated by absorption, can follow a true attractive inverse square law from near to far-field separation distances.

Direct observation of dynamic tube dilation in entangled polymer blends: a combination of neutro scattering and dielectric techniques.

Malo de Molina P, Alegría A, Allgaier J, Kruteva M, Hoffmann I, Prévost S, Monkenbusch M, Richter D, Arbe A, and Colmenero J
Physical Review Letters 123, 187802 (2019)

An open question on the dynamics of entangled polymers is how the topological constraints are released by mobile neighboring chains or, in other words, how the constraining 'tube' is dilated. This work by members of the Polymers & Soft Matter group (in collaboration with Forschungszentrum Jülich, Germany and Institut Laue-Langevin, France) reports the direct microscopic observation of the time-dependent tube dilation in iso-frictional blends.

Polymeric materials are ubiquitous in every-day life. Their mechanical performance, industrial processing and other end-use properties are determined by their dynamics. Hence, it is important to fundamentally understand how the macromolecules move in the material, in particular in modern materials with increased complexity.

Nowadays, it is well accepted that the viscoelastic properties of high molecular weight polymer melts are controlled by entanglements: topological constraints imposed by mutually interpenetrating and uncrossable polymer chains. In the tube model for entangled chains, these constraints are represented by a fictitious tube that restricts the lateral motion of the polymer chain within its diameter leading to a reptation motion of the chain along the tube.

However, the pure reptation tube model fails in real materials, which are polydisperse and most times multicomponent. In these cases other mechanisms compete with reptation, mainly, contour length fluctuations (CLF) —fluctuations of the length of the tube— and constraint release (CR) —probe relaxation driven by the motions of surrounding chains. CR becomes particularly important in polydisperse melts and binary blends, especially where long polymer chains are mixed with short additives of the same chemistry (iso-frictional blends) but sometimes of different polymer architecture. A simplified model of the many-body CR mechanism, called dynamic tube dilation (DTD), considers that CR leads to an increase with time of the tube diameter. The effective terminal tube dilation of the long chains in polymer blends can be determined by obtaining the long-time tube diameter from macroscopic techniques such as dielectric spectroscopy (DS) and rheology. However, these techniques cannot resolve the time evolution of the tube diameter involved in the dilation phenomenon.

This work exploits the spatial and time resolution of neutron spin echo (NSE) to directly probe the time-dependent tube dilation in model blends based on polyisoprene with different topologies: short linear chains and small star polymers blended with long linear entangled chains. The smaller additives have faster dynamics that affect the tube dynamics of the longer chains and enhance the mechanism of CR.

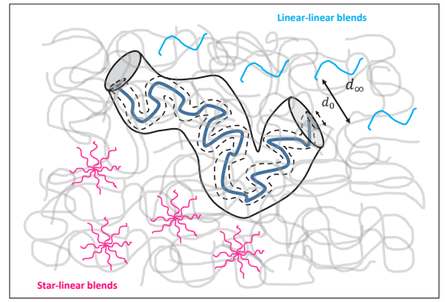


Figure 1. Schematic representation of the tube dilation in linear-linear and star-linear blends. The undilated tube has a diameter d_0 and increases with time to d_∞ as a consequence of CR.

Combination with rheology and dielectric spectroscopy reveals the additive terminal time as that governing tube dilation

Neutron spin echo provides unique evidence at molecular scale of time-dependent constraints removal

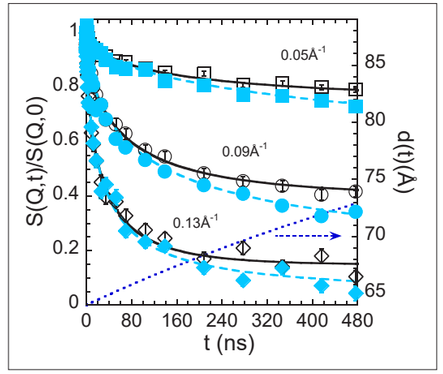


Figure 2. Time evolution of the chain dynamic structure factor measured by NSE for the long chains in the pure matrix (black) and in the blends with short linear polymer (blue). The dotted line shows the increase of the tube diameter in the blend as the time increases.

First, by means of DS in the terminal range we confirmed a dilated tube mechanism for the long chains relaxation. Second, we demonstrated that the time-dependent tube dilation can be directly inferred from the NSE data (see Figure 2). It shows itself in an additional time dependence of the dynamic structure factor in the local reptation regime. Moreover, by combining the NSE study with rheology and dielectric spectroscopy on the additive, the characteristic time that governs tube dilation was identified as the terminal time of the additive. This finding will help elucidate the mechanism for constraint release and, thus, will facilitate the design of polymeric materials with the desired rheological properties.

DIPC HIGHLIGHT 2019

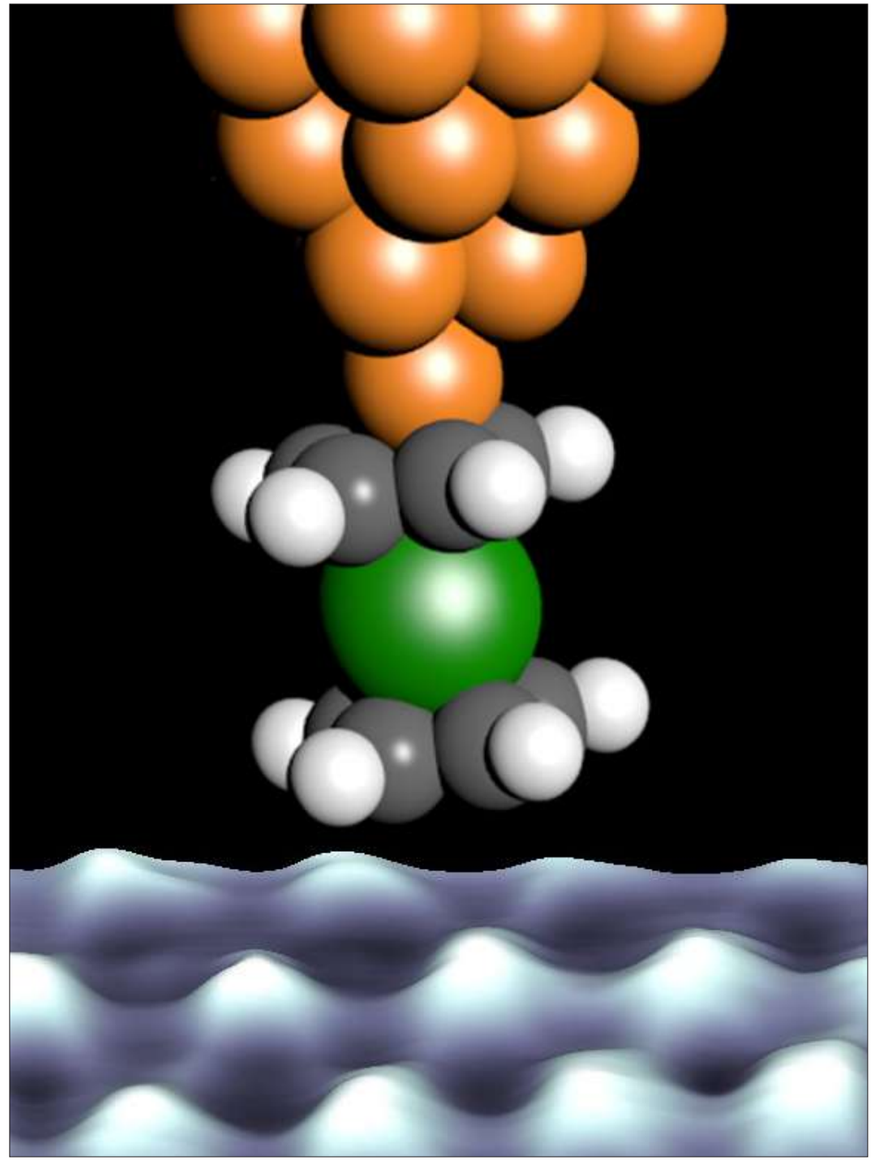
Atomic-scale spin sensing with a single molecule at the apex of a scanning tunneling microscope

Verlhac B, Bachellier N, Garnier L, Ormaza M, Abufager P, Robles R, Bocquet ML, Ternes M, Lorente N, and Limot L
Science 366, 623-627 (2019)

An international team led by Laurent Limot (Strasbourg), Markus Ternes (Jülich) and Nicolás Lorente, researcher at CFM and Donostia International Physics Center (DIPC) has shown that minute magnetic fields can be detected using a magnetic molecule that is scanned along a surface. The scanning is made displacing the molecule on a metallic tip such that the displacements are sub-atomic and an electronic current is passed between tip and studied substrate. The small displacements are key to obtaining very high resolution but the new aspect of the work is to use a magnetic excitation of the molecule when electrons flow through it. The magnetic excitation can easily be perturbed by the substrate yielding precious information on its magnetic structure.

The authors of the recent publication in Science specially crafted the tip apex to bring a novefunction to the sharp tip: They made it sensitive to magnetic moments by placing a quantum molecular magnet containing a single Nickel atom. The molecule is shown in the figure in the configuration gleaned from geometrical studies mainly using calculations. The ground state of the molecule corresponds to a molecular magnetic moment parallel to the substrate surface. The molecule has a low-energy excitation of roughly 4 meV that corresponds to directing the magnetic moment perpendicular to the surface. The spin of this molecule is S=1 and is preserved in the depicted configuration. The excitation is easily performed by the flowing electrons in the figure's set up because each electron efficiently undergoes a splin flip while exciting the molecular spin, to preserve the system's total spin. The excitation opens a new conduction channel leading to a jump in the differential conductance of the molecular junction that is revealed in the measurements. This jump takes place at the bias matching the excitation energy. When the molecule is close to a magnetic object, the excitation energy changes due to the new magnetic excitations. As a consequence, the magnetic properties of the surface can be studied with sub-atomic resolution.

There are two important aspects of this work; First, the use of a molecule as active sensor makes it very reproducible and easy to implement in instruments used by other groups world-wide working in the field. Second, the detection scheme relies only on easily observable properties in the sensor tip and "dark" magnetic moments, which are usually difficult to measure, become accessible. In summary, with this work scientists have expanded their nanoscale toolbox with a new tool sensitive to the magnetic properties which will be important for future applications ranging from nanoscale memory-devices to novel materials or applications in the field of quantum simulation and computing.



A molecule at the tip of the tunneling microscope is the key to achieving unprecedented accuracy of magnetic detection on an atomic scale

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374 Thermal, electric and spin transport in superconductor/ferromagnetic-insulator structures.
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375 Work statistics, loschmidt echo and information scrambling in chaotic quantum systems.
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377 The route to massive black hole formation via merger-driven direct collapse: a review.
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378 Colloquium: Atomic spin chains on surfaces.
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379 Tunable upconversion emission in $NaLuF_4$-glass-ceramic fibers doped with Er^{3+} and Yb^{3+}.
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380 Spin-layer locked gapless states in gated bilayer graphene.
Jaskolski W, and Ayuela A.
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381 In silico design of mimosine containing peptides as new efficient chelators of aluminum.
Mujika JI, Dalla Torre G, Lachowicz JI, and Lopez X.
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382 Atomic-scale spin sensing with a single molecule at the apex of a scanning tunneling microscope.
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383 Silicic acid: the omniscient molecule.
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Science of the Total Environment 665, 432 (2019).

384 Solution blow spinning of polymer/nanocomposite micro-/nanofibers with tunable diameters and morphologies using a gas dynamic virtual nozzle.
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385 Rich magnetic quantization phenomena in AA bilayer silicene.
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Mendoza-Arenas JJ, Gomez-Ruiz FJ, Rodriguez FJ, and Quiroga L.
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390 Peculiar optical properties of bilayer silicene under the influence of external electric and magnetic fields.
Do TN, Gumbs G, Shih PH, Huang DH, Chiu CW, Chen CY, and Lin MF.
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391 Conditions for fully gapped topological superconductivity in topological insulator nanowires.
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392 Scattering of microwaves by a passive array antenna based on amorphous ferromagnetic microwires for wireless sensors with biomedical applications.
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393 Isolation of cyclic penta(ethylene oxide) from mixtures with its linear analog by combining selective intercalation into graphite oxide and solvent approaches.
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394 Direct imaging of the induced-fit effect in molecular self-assembly.
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395 Numerical modelling of non-ionic microgels: an overview.
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396 Pnicogen and tetrel bonds-tetrahedral Lewis acid centres.
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397 Optical helicity and optical chirality in free space and in the presence of matter.
Poulikakos LV, Dionne JA, and Garcia-Etxarri A.
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398 Performance of the NOF-MP2 method in hydrogen abstraction reactions.
Lopez X, and Piris M.
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399 Kinetics of the condensation reaction of urea and furfural in a heterogeneous phase leading to difurfurylidenetriurea: a calorimetric study.
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400 Effect of molecular weight on vitrification kinetics and molecular mobility of a polymer glass confined at the microscale.
Monnier X, and Cangialosi D.
Thermochimica Acta 677, 60 (2019).

401 Electron spill-out effects in plasmon excitations by fast electrons.
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Book Chapter

Novel aspects of element-element bonds in main group chemistry.
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DIPC COMMUNITY

Pictured here is part of the DIPC Community
at the headquarters in Donostia / San Sebastián.

DIPC HEADQUARTERS
DONOSTIA / SAN SEBASTIÁN

Researchers

DIPC Associates

Prof. Javier Aizpurua CSIC
Dr. Maite Alducin CSIC
Dr. Ignacio Arganda-Carreras UPV/EHU
Prof. Andrés Arnau UPV/EHU
Prof. Emilio Artacho CIC nanoGUNE
Dr. Andrés Ayuela, CSIC
Prof. Rolindes Balda UPV/EHU
Dr. Sara Barja UPV/EHU
Dr. Aitor Bergara UPV/EHU
Dr. Sebastian Bergeret CSIC
Dr. Maria Blanco UPV/EHU
Dr. Tom J. Broadhurst UPV/EHU
Dr. Igor Campillo Euskampus
Dr. Daniele Cangialosi CSIC
Dr. Miguel Angel Cazalilla CSIC
Dr. Silvina Cerveny CSIC
Dr. Deung-Jang Choi MPC
Prof. Eugene Chulkov UPV/EHU
Dr. Martina Corso CSIC
Prof. Fernando Cossio UPV/EHU
Dr. David De Sancho UPV/EHU
Dr. Asier Eiguren UPV/EHU
Dr. Ion Errea UPV/EHU
Prof. Joaquín Fernández UPV/EHU
Dr. Elena Formoso UPV/EHU
Dr. Idoia García de Gurtubay UPV/EHU
Dr. Vitaly Golovach CFM
Dr. Miguel Angel Gosálvez UPV/EHU
Dr. Elisa Jiménez-Izal UPV/EHU
Dr. Iñaki Juaristi UPV/EHU
Dr. Stefan Kurth UPV/EHU
Dr. Aritz Leonardo UPV/EHU
Dr. Xabier López UPV/EHU
Dr. Nicolás Lorente CSIC
Dr. Jon M. Matxain UPV/EHU
Dr. Jose M. Mercero UPV/EHU
Prof. Gabriel Molina Terriza MPC
Dr. Angel Moreno CSIC
Prof. Enrique Ortega UPV/EHU
Dr. Mikhail Otrokov CFM
Prof José Ignacio Pascual nanoGUNE
Prof. Juan Ignacio Pérez UPV/EHU
Prof. José Maria Pitarke UPV/EHU
Prof. Yuri Rakovich UPV/EHU
Dr. Elixabete Rezabal UPV/EHU
Prof. Alberto Rivacoba UPV/EHU
Dr. Celia Rogero CSIC
Prof. Ángel Rubio UPV/EHU
Dr. Daniel Sánchez Portal CSIC
Dr. Ane Sarasola UPV/EHU
Dr. Frederik Schiller CSIC
Dr. Gustavo Ariel Schwartz CSIC
Prof. Ivo Souza UPV/EHU
Dr. Ilya Tokatly UPV/EHU
Dr. Geza Toth UPV/EHU
Prof. Jesus M. Ugalde UPV/EHU
Prof. Lucia Vitali UPV/EHU
Dr. Nerea Zabala UPV/EHU

Ikerbasque Research Professors

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

Prof. Andrey Kazansky
01/01/2012–Present
Investigation of subfemto atto second processes in gases and solids caused by ultrashort laser pulses. Investigation of dynamics of electrons in suface and image states of noble metal and their interaction with adsorbates.

Prof. Eugene Krasovskii
01/01/2012–Present
Electronic structure of nanosystems, surfaces and interfaces. Attosecond time resolved photoelectron spectroscopy to study the dynamics of electronic excitations. Full dielectric function of bulk crystals, surfaces and two dimensional nanostructures. Development of new computational methods of the density funtional theory.

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

Prof. 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.

Prof. 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.

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

Prof. Geza Giedke
01/09/2014–Present
Quantum Information and Quantum Optics: Implementations of QIP in atomic and solid-state systems.

Prof. Dimas García de Oteyza Fieldman
01/05/2015–Present
Physical chemistry phenomena in organic materials and organic-inorganic interfaces.

Prof. Juan José Sáenz Gutiérrez
01/09/2015–Present
Light scattering in colloidal suspensions.

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

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

Ikerbasque Research Associates

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

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

Prof. Roman Orus Lacort
01/09/2018–Present
Quantum information and condensed matter.

Prof. Adolfo Del Campo Echevarria
01/01/2019–Present
Quantum science and technology and quantum non-equilibrium dynamics.

Prof. Rafael Yuste Rojas
26/03/2019–Present
Neurophysics.

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

Senior Position

Dr. Irina Sklyadneva
14/05/2003–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).

Dr. Marek Grzelczak
01/09/2017–Present
Synthesis and self-assembly of plasmonic nanoparticles for photochemical applications.

Dr. Arantzazu Garcia Lekue
01/11/2017–Present
Modeling electron transport at the nanoscale. Theoretical investigation of electron processes at nanostructured surface.

Dr. Paola Ferrario
01/12/2017–Present
Neutrino physics.

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

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

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

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

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

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

Ikerbasque Research Fellows

Dr. Dario Bercioux
01/10/2019–30/09/2019
Quantum transport in nanostructures.

Dr. Rubén Esteban Llorente
29/11/2016–Present
Quantum plasmonics.

Dr. Maia García Vergniory
01/01/2018–Present
Prediction of new topological phases and materials.

Dr. Eduard Matito Gras
15/02/2018–Present
Development of electronic structure methods and real-space descriptors of chemical bonding and aromaticity.

Dr. Santiago Blanco Canosa
01/10/2019–30/09/2019
Synchrotron research in high Tc superconductors and low dimensional ferromagnets.

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

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

Dr. Aurelia Chenu
01/01/2019–Present
Nonequilibrium quantum dynamics in open systems. Many body description of nano structures.

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

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

Fellows Gipuzkoa

Dr. Aitzol Garcia Etxarri
01/11/2014–31/10/2019
Nanophotonics theory.

Postdoctoral Positions

Dr. Miren Iosune Arrastia Basalo
01/08/2013–Present
Multiple spin state reactivity in Fe-containing complexes and enzymes.

Dr. Carlos García Fernandez
20/04/2016–14/01/2019
Development of transport methods based on Wannier function.

Dr. Jon Iñaki Mujika
16/08/2016–15/08/2019
Molecular dynamics of membrane structure.

Dr. Aleksander Victorovich Terentjev
01/09/2016–31/08/2019
Time dependent density functional theory beyond the local density approximation.

Dr. Jorge Budagosky Marcilla
01/10/2016–30/09/2019
Computational solid state spectroscopy.

Dr. Rafael Grande Aztatzi
13/03/2017–Present
Molecular dynamics of Al protein interactions.

Dr. Pedro Brandimarte Mendonça
01/10/2017–Present
Electronic structure and quantum transport in graphene based nanostructures and networks.

Dr. Xavier Monnier
15/11/2017–Present
Ultra dense/low energy state glasses by agin nanostructured polymers.

Dr. Paula Malo de Molina Hernández
15/12/2017–30/06/2019
All polymer nano composites: effect of soft nano objects on polymer structure and dynamics.

Dr. Daniel José Arismendi Arrieta
05/02/2018–Present
Coarse grained molecular dynamics simulations of soft nanoparticles as stabilizers for Pickering emulsions.

Dr. Alessio Terenzi
01/03/2018–31/12/2019
Developing innovative photoactivatable gold complexes that can be used as effective prodrugs for photochemotherapy and simultaneously act as imaging agents.

Dr. Abel Carreras Conill
01/04/2018–Present
Development of electronic structure methods for excited states.

Dr. Andrew Weber
17/05/2018–Present
Magnetic properties of nanostructured surface alloys and interfaces.

Dr. Miguel Varga
21/06/2018–Present
Quantum control of nanostructures.

Dr. Matteo Zennaro
01/07/2018–Present
Cosmological structure formation.

Dr. Giuseppe Foti
01/09/2018–31/08/2019
Current induced vibrational instabilities in GNR based nanogaps.

Dr. Francesc Monrabal Capilla
01/09/2018–30/06/2019
Development of xenon detectors for basic and applied physics.

Dr. Maria Sanroman Iglesias
01/09/2018–Present
Plasmon based colorimetric biosensors for liquid biopsy.

Dr. Alvaro Martínez Ceballos
10/09/2018–Present
Bioorthogonal Photocatalytic Activation of Metal-Based Prodrugs.

Dr. Mohammad Ali Aboudzadeh
01/10/2018–Present
Metal/cyclic hybrid materials for biomedical applications.

Dr. Ivan de Martino
01/10/2018–Present
Dark matter theory and predictions.

Dr. Marcos Pellejero Ibañéz
01/10/2018–Present
Cosmological N-body simulations and the analysis of the large-scale structure of the universe.

Dr. Tineke Van den Berg
01/10/2018–Present
Spectral and transport properties of pseudo-spin one systems.

Dr. Yuan Zhang
02/10/2018–01/10/2019
Coherent effects in plasmon molecule interactions.

Dr. Sergio Contreras Hantke
04/10/2018–Present
Modelling of galaxy formation physics and its impact on clustering and cosmological parameters.

Dr. Yetli Rosas Guevara
26/10/2018–Present
Theory and observation of galaxy formation.

Dr. Eduardo Duque Redondo
01/11/2018–30/09/2019
Atomistic simulations of clays and cement based materials: transport properties.

Dr. Thomas Hendel
01/11/2018–Present
Electronic coupling in semiconductors metal hybrid systems.

Dr. James Lawrence
03/12/2018–Present
Functional materials synthesized by surface supported chemistry under vacuum.

Dr. Ivan Rivilla De la Cruz
01/01/2019–Present
Computational and physical chemistry.

Dr. Jon Zubeltzu Sesé
01/01/2019–Present
Nanoclusters of semiconducting compounds in ionic liquids.

Dr. Eloy Ramos Cordoba
04/01/2019–31/07/2019
Development of density functional approximations.

Dr. Jie Hou
20/02/2019–Present
Interfaces between two dimensional systems.

Dr. Ilya Nechaev
01/03/2019–31/10/2019
Linear response, low-energy electron scattering, and photoemission within the relativistic k.p methodology.

Dr. Luis Alejandro Miccio
15/03/2019–25/09/2019
Dynamics of polymers and biopolymers- combining experimental and numerical approaches.

Dr. Seyed Saeed Soyouf Jahromi
18/03/2019–Present
Tensor network methods for quantum many body systems.

Dr. Marcelo José Ambrosio
25/03/2019–Present
Theoretical description of photoemission processes at the attosecond scale.

Dr. Wen Wan
11/04/2019–Present
Growth and characterization of 2D materials and related heterostructures.

Dr. Rodrigo Ezequiel Menchón Turco
01/05/2019–Present
Vibrational properties of carbon-based nanostructures.

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

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

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

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

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

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

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

PhD Students

Néstor Merino Díez
01/09/2015–31/08/2019
Functional materials synthesized by surface-supported chemistry under vacuum.

Bogusz Bujnowski
01/04/2016–30/11/2019
Quantum transport in hybrid structure with semimetals, excitonic insulators and superconductor.

Jordan Ochs
01/10/2016–Present
Synthesis of cyclic polymers.

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

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

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

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

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

Moritz Müller
09/06/2017–31/07/2019
Lifetimes of HOMO and LUMO states of organic molecules relevant for organic photovoltaics on different substrates.

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

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

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

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

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

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

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

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

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

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

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

Julie Baumard
15/04/2018–Present
Superconducting hybrid strcutures with spin-dependent fields.

Quentin Schaeverbeke
15/04/2018–Present
Dynamical aspects of quantum transport in nanoelectronics.

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

Giovanni Arico
01/07/2018–Present
Cosmological implications of dark energy.

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

Rodrigo Castrillo Bodero
01/10/2018–31/07/2019
Exotic magnetism and electron correlation phenomena at the interface of rare-earth based materials and molecular overlayers.

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

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

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

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

Mikel Iraola Iñurrieta
01/11/2018–31/05/2019
Electronic correlations and thermalstapility in topological materials.

Ignacio Piquero Zulaica
01/11/2018–31/03/2019
Angle resolved photoemission from boron nitride nanostripes.

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

Laura Filomena Mazzei
02/11/2018–Present
Bioorthogonal photoredox catalysis for cancer therapy.

Martín Molezuelas Ferreras
07/11/2018–30/06/2019
Quantum Nanophotonics.

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

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

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

Andrei Bylinkin
09/01/2019–06/10/2019
Optical phenomena in novel Van der Waals materials.

Gonzalo Diaz Lopez
14/01/2019–30/05/2019
Support for NEXT project.

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

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

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

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

Research Assistants

Jordi Torrent Collell
16/06/2018–Present

Alberto Martínez Perez
01/11/2018–Present

Beatriz Romeo Zaragozano
01/11/2018–Present

Daniel Cubero Mimbiela
05/11/2018–Present

Lourdes Ondaro Mallea
02/09/2019–Present

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

Leonce Dupays
07/10/2019–Present

Internships

Miryam Martínez Vara
Universidad de Valencia, Spain
05/11/2018–30/09/2019
Studies to identify Ba ++ / Ra ++ ions using the technique SMFI (single molecule fluorescence imaging).

Albert Johannes Pool
Universiteit Utrecht, Netherlands
04/02/2019–11/06/2019
Quantum engenieering in topological insulators.

Oxana Azpitarte Aguirre
UPV/EHU, Donostia/San Sebastián, Spain
01/06/2019–31/07/2019
Development of new photoactivatable anticancer prodrugs.

Nathaniel Capote Robayna
Universidad de Oviedo, Spain
01/06/2019–31/07/2019
Theory project: 2D nanophotonics.

David Silva Brea
UPV/EHU, Donostia/San Sebastián, Spain
01/06/2019–31/07/2019
Study of the oxidation states of aluminum in different environments.

Andoni Ugartemendia Biurrun
UPV/EHU, Donostia/San Sebastián, Spain
01/06/2019–31/07/2019
Doping of Pt-based nanocatalysts for their use in CO oxidation.

Iñigo Gómez Tapia
UPV/EHU, Donostia/San Sebastián, Spain
03/06/2019–31/07/2019
Publication analysis system based on relational database.

Sergio Hurtado Solorzano
UPV/EHU, Leioa, Spain
03/06/2019–31/07/2019
Development of a VPN to improve the security in the access to DIPC supercomputers.

Alexia Tialiou
Aristotle University of Thessaloniki, Greece
03/06/2019–30/08/2019
Development of photoactivatable anticancer agents.

Itsaso Blanco González
University College London, UK
10/06/2019–09/08/2019
Quantum transport in nanoscale devices.

Asier Rodríguez Escalante
UPV/EHU, Leioa, Spain
10/06/2019–09/08/2019
Quantum transport in nanoscale devices.

Imanol Echeverría Franco
UPV/EHU, Leioa, Spain
19/06/2019–18/08/2019
Development of open-source computer vision tools for biomedical microscopy data.

Andoni Agirre Arabolaza
UPV/EHU, Leioa, Spain
20/06/2019–20/08/2019
Infrared Light Control in materials at the nanoscale.

Martín Irizar Landa
UPV/EHU, Facultad de Ciencias, Leioa, Spain
20/06/2019–19/08/2019
Interference effects and thermal transport in graphene nanostructures.

Lourdes Ondaro Mallea
UPV/EHU, Leioa, Spain
24/06/2019–24/08/2019
Computational cosmology and the large scale structure of the universe.

José Polo Gómez
Universidad Complutense de Madrid, Spain
01/07/2019–31/08/2019
Strong coupling effects in plasmon-molecule systems.

Macià Mut Sbert
Universidad de Barcelona, Spain
02/07/2019–31/08/2019
Electronic structure in optoelectronics.

Nina Tarnowicz
Wroklaw University of Science and Technology, Wrocław, Poland
07/07/2019–07/09/2019
All metal photocatalysis.

Jack James Mayo
Unversity of Groningen, Faculty of Mathematics and Natural Sciences,
Groningen, Netherlands
09/07/2019–01/09/2019
Nonadiabatic quantum computation and full counting statistics of topological defects.

Andrea Rogolino
Università di Padova, Italy
10/07/2019–07/09/2019
Aplication of plasmonic nanoparticles in photocatalitic applications.

Alonso Campos Hernández
Universsity of Cambridge, UK
15/07/2019–15/09/2019
Photocurrents in magnetic semiconductors.

Mateusz Staniak
Warsaw University of Technology, Poland
20/07/2019–17/09/2019
Machine learning in nanotechnologies.

Andrei Paulau
Technical University of Münich, Germany
01/08/2019–30/09/2019
A real space model of strong correlation.

Lea Kokott
Faculty of Physics in Geowissenschaten, Leipzig, Germany
26/08/2019–01/11/2019
Topological systems in the presence of correlated disorder.

All Researchers as of 31/12/2019

Special Assignments

Arantzazu Garcia Lekue
DIPC Calls for Young Researchers

Luca Salassa
DIPC Workshops and DIPC Schools

Geza Giedke and Thomas Frederiksen
DIPC Colloquia

Marek Grzelczak
DIPC Seminars

Deung-Jang Choi and Nicolás Lorente
DIPC Courses

Aitzol García Etxarri
DIPC Transdisciplinary Skills Courses

Fabienne Barroso and Rubén Esteban
DIPC Summer Internships

Gender Equality Committee

Aitzol García Etxarri

Amaia Arregi

Ana López de Goicoechea

Beatriz Suescun

David de Sancho

Elisa Jiménez Izal

Irene Ruiz Ortiz

Luz Fernández

Maia García Vergniory

Ricardo Díez Muiño

Silvia Bonoli

Visiting Researchers

Long visits

Prof. Alexandre Reily Rocha
Institute for Theoretical Physics,
State University of São Paulo, Brazil
16/01/2019–15/02/2019
Electron phonon interactions and transport indisordered systems.

Prof. Young Rok Jang
Incheon National University, Incheon,
South Korea
01/01/2018–28/02/2019
Simulation of magnetic properties of surfaces and adsorbates.

Prof. Ziya Aliyev
Azerbaijan State Oil and Industry University,
Baku, Azerbaijan
04/01/2019–01/03/2019
Material physics of topological insulators.

PhD student Federica Guarra Lumare
Universitá de Pisa, Italy
15/01/2019–31/03/2019
Development of photoactivatable anticancer agents.

PhD student Miriam Kosik
Nicolaus Copernicus University, Toruń, Poland
19/01/2019–17/02/2019
Manipulating emission rates and interactions of quantum emitters beyond electric dipole approximation.

PhD student Meilani Wibowo
Zernike Institute for Advanced Materials,
University of Groningen, Netherlands
21/01/2019–31/03/2019
Combined restricted active space configuration interaction with short range density functional theory for the Study of excitation and electron transfer processes.

Prof. Vito Despoja
Institute of Physics, Zagreb, Croatia
31/01/2019–28/02/2019
Strong 2D plasmons in alkali metal intercalated graphene on Ir(111).

Dr. Roman Kuzian
Institute for Problems of Materials Science
National Academy of Sciences of Ukraine,
Kiev, Ukraine
01/02/2019–30/04/2019
Time-resolved photoemission from solids.

Prof. Antonio Hernando Grande
Universidad Complutense de Madrid,
Instituto de Magnetismo Aplicado, Madrid, Spain
05/02/2019–05/04/2019
Effect of magnetic fields on gating
of neuron channels.

Prof. Joseph Richard Manson
Clemson University, Clemson,
South Carolina, USA
08/02/2019–15/03/2019
Electron-phonon interactions near surfaces.

PhD student Tangyou Huang
Shanghai University, Shanghai, China
16/02/2019–15/05/2019
Reseach related with quantum phase transition.

PhD student Jingjun Zhu
Shanghai University, Shanghai, China
16/02/2019–15/05/2019
Theoretical work about many-body system.

Prof. Oleg Dolgov
Lebedev Physical Institute, Russian Academy
of Science, Moscow, Russia
01/03/2019–30/06/2019
Electronic excitations and superconducting
instability in solids.

PhD student Farihah Haque
Tulane University, New Orleans, Louisiana, USA
01/03/2019–30/04/2019
Cyclic polymers.

Prof. Luis Alberto Montero Cabrera
Universidad de La Habana,
La Habana, Cuba
31/03/2019–30/04/2019
Machine learning applied to predict
molecular spectra.

Prof. Wolfgang Schattke
Institut für Theoretische Physik und Astrophysik,
Christian-Albrechts-Universität zu Kiel, Germany
01/04/2019–31/05/2019
Molecular machines on surfaces:
Nanonmechanical properties
of small molecules.

Prof. Vladlen Zhukov
Institute of Solid State Chemistry of the Russian
Academy of Sciencies, Ekaterinburg, Russia
08/04/2019–08/06/2019
Electronic band structure and phisico-chemical
properties of cobaltites and molibdates
with the double perovskite structure.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
02/05/2019–31/05/2019
Surface electron-phonon interaction.

PhD student Nicolò Orsoni
Università di Parma, Italy
02/05/2019–02/11/2019
Development of photoactivatable
anticancer agents.

Prof. Andrés Felipe Santander Syro
Université Paris-Sud, CSNSM, Orsay, France
02/05/2019–02/09/2019
Electronic structure of exotic states at the
surface of correlated materials: coupled
STM-ARPES studies.

PhD student Adeleh Vatankhahan
Shahrood University of Technology,
Semnan, Iran
02/05/2019–31/10/2019
Electronic and transport properties
of graphene-based nanostructures.

Prof. Vladimiro Mújica Hernandez
Arizona State University, Tempe, Arizona, USA
04/05/2019–15/08/2019
Theoretical and computational models
for Chirality-Induced Spin Polarization (CISP)
effect in spin-dependent chemistry
and solid state NMR.

PhD student Diego Romero Abujetas
Instituto de Estructura de la Materia (IEM-CSIC),
Madrid, Spain
09/05/2019–09/06/2019
Theory of light scattering in nano-structured
highly refractive media.

PhD student Abhijit Chaudhari
Indian Institute of Technology,
Uttar Pradesh, India
11/05/2019–15/08/2019
Control of quantum critical dynamics in chains.

Prof. Barry Bradlyn
University of Illinois at Urbana-Champaign,
Urbana, USA
15/05/2019–15/06/2019
Topological photonics, Interacing topological
quantum chemistry.

Prof. Oleg V. Prezhdo
University of Southern California,
Los Angeles, USA
21/05/2019–27/08/2019
Modeling of excitation dynamics in nanoscale
materials using time-domain density functional
theory and advanced techniques.

PhD student Oscar Pozo Ocaña
Instituto de Ciencia de Materiales de Madrid,
Spain
27/05/2019–28/06/2019
Photocurrents in magnetic materials depending
on light polarization.

Prof. Juan Faustino Aguilera Granja
Instituto de Física, Universidad Autónoma
de San Luis Potosí, México
01/06/2019–31/07/2019
Electronic properties of 2-dim nanostructures.

Dr. Maxim Kharitonov
Theoretical Physics IV, University of Würzburg,
Germany
01/06/2019–30/09/2019
Bound states in topological systems.

Prof. Fernando Martín García
Universidad Autónoma de Madrid and IMDEA
Nanociencia, Madrid, Spain
01/06/2019–30/06/2019
Attosecond physics in condensed
matter systems.

Prof. Vladimir Nazarov
Research Center for Applied Sciences,
Academia Sinica, Taipei, Taiwan
01/06/2019–30/06/2019
Dielectric response in photoemission.

Prof. Andrey Vasenko
National Research University Higher School
of Economics, Moscow, Russia
01/06/2019–31/08/2019
Superconductivity in topologically nontrivial
materials.

PhD student Jonas Lundholm Bertelsen
DTU, Technical University of Denmark,
Copenhagen, Denmark
03/06/2019–26/07/2019
Transport in nanostructures.

Dr. Tatiana Menshchikova
Tomsk State University, Tomsk, Russia
05/06/2019–31/08/2019
Investigation of the electronic structure
of topological insulators using first-principles
calculations.

Dr. Igor Rusinov
Tomsk State University, Tomsk, Russia
05/06/2019–31/08/2019
Investigation of the Weyl Semimetal,
topologically non trivial systems using
first-principles and model calculations.

Prof. Frank Scheffold
University of Fribourg, Fribourg, Switzerland
07/06/2019–31/08/2019
Light transport in correlated media.

Prof. Francisco José García Vidal
Universidad Autónoma de Madrid, Spain
10/06/2019–31/07/2019
Valley polaritonics in 2D materials.

Prof. Carmen Mijangos Ugarte
Consejo Superior de Investigaciones Científicas, Instituto de Ciencia y Tecnología de Polímeros, Madrid, Spain
10/06/2019–09/08/2019
Challenges in polymer nanotechnology: chemical strategies and cofinement effects.

Prof. Hanan Basioni Ahmed Awd Allah
Faculty of Science, Helwan University, Cairo, Egypt.
17/06/2019–12/12/2019
Treatment textile industrial wastewater from organic pollutants by using mono-, bi- and tri-metallic nanostructures of silver, gold and palladium metals.

Prof. Pavel Jelínek
Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic
23/06/2019–26/07/2019
Molecules at surfaces.

Prof. Edvin Lundgren
Institute of Physics, Lund University, Lund, Sweden
24/06/2019–11/08/2019
Chemical reactions at curved surfaces.

Prof. Pablo Artal Soriano
Laboratorio de Óptica, Universidad de Murcia, Spain
01/07/2019–31/07/2019
Biomedical optics and photonics.

Prof. Andrey Borissov
Institute of Melecular Science in Orsay, CNRS, Université París-Sud, Orsay Cedex, France
01/07/2019–30/08/2019
Quantum plasmonics.

Prof. Miguel Angel Cazalilla Gutierrez
National Tsing Hua University Taiwan, Hsinchu City, Taiwan
01/07/2019–31/08/2019
Spin transport in low dimensional systems.

Prof. Javier García de Abajo
ICFO-Instituto de Ciencias Fotónicas, Castelldefels, Barcelona, Spain
01/07/2019–31/07/2019
Plasmons in atomically thin metal films.

Prof. Francisco Guinea López
Imdea Nanoscience, Madrid, Spain
01/07/2019–31/07/2019
Two dimensional materials.

Prof. Pilar Hernández Gamazo
Instituto de Física Corpuscular CSIC-UV, Valencia, Spain
01/07/2019–31/07/2019
Outlook in neutrino physics.

Prof. Maria Angeles Hernández Vozmediano
Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain
01/07/2019–31/07/2019
Topological matter.

Prof. Antonio Hernando Grande
Universidad Complutense de Madrid, Instituto de Magnetismo Aplicado, Madrid, Spain
01/07/2019–31/10/2019
Effect of magnetic fields on gating of neuron channels.

Prof. Nikolay Kabachnik
CFEL DESY, Hamburg, Germany
01/07/2019–30/09/2019
Theoretical study of Auger processes excited by x-rays in presence of optical or THz field.

Prof. Luis Martin Moreno
Instituto de Física de Materiales de Aragón, Universidad de Zaragoza, Spain
01/07/2019–31/07/2019
Theoretical nanophotonics.

Prof. Vasily Stolyarov
Moscow Institute of Physics and Technology, Dolgoprudny, Russia
01/07/2019–01/08/2019
Investigation of the coexistence of superconductivity and ferromagnetism on the atomic scale.

Prof. Darrin M. York
Laboratory for Biomolecular Simulation Research, Center for Integrative Proteomics Research, Rutgers University, Piscataway, New Jersey, USA
01/07/2019–29/07/2019
Simulation of biological systems.

Prof. Michael Rappaport
Weizmann Institute o Science, Faculty of Physics, Rehovot, Israel
15/07/2019–30/08/2019
PETALO.

PhD student Ermolaev Giorgii
MIPT, Dolgoprudny, Russia
21/07/2019–31/08/2019
Graphene plasmonics.

PhD student Kirill Voronin
Moscow Institute of Physics and Technology (National Research University), Dolgoprudny, Russia
21/07/2019–31/08/2019
Graphene plasmonics.

Prof. Matthew Gilbert
University of Illinois and Stanford University, California, USA
22/07/2019–26/08/2019
Applied topology in photonic and other non-condensed matter systems.

Prof. Eugene Kogan
Bar-Ilan University, Ramat-Gan, Israel
25/07/2019–24/08/2019
Kondo effect in graphene.

Prof. Bo Hellsing
Gothenburg University, Sweden
01/08/2019–30/09/2019
Electron phonon coupling in low dimensional systems.

Prof. Vladimir Kuznetsov
National Research Tomsk State University, Tomsk, Russia
01/08/2019–31/08/2019
Topological insulators.

Prof. Ceferino López Fernández
Instituto de Ciencia de Materiales, CSIC, Madrid, Spain
31/08/2019–29/09/2019
Disorder photonics.

Prof. Peter Saalfrank
Institut für Chemie, Universität Postdam, Postdam-Golm, Germany
01/09/2019–31/10/2019
Nonadiabatic molecular dynamics of laser-driven processes at surfaces.

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

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

PhD student Yutaro Goto
Osaka Prefecture University, Osaka, Japan
04/09/2019–28/11/2019
Light scattering and optical forces.

Prof. Alberto Galindo
Facultad de Física, Universidad Complutense, Madrid, Spain
06/09/2019–14/10/2019
Finishing touches on my book "Quantum Mechanics".

Prof. Joseph Richard Manson
Clemson University, Clemson, South Carolina, USA
16/09/2019–31/10/2019
Electron-phonon interaction at surfaces.

Dr. Magdalena Marganska-Lyzniak
Institute for Theoretical Physics, University of Regensburg, Germany
22/09/2019–23/10/2019
Topological states at domain boundaries in honeycomb lattices.

PhD student Shiue-Yuan Shiau
Physics Division, National Center for Theoretical Sciences, Hsinchu, Taiwan
30/09/2019–31/10/2019
Microscopic origin of decoherence in SC qubits.

Prof. Julio Alonso Martín
Facultad de Ciencias, Universidad de Valladolid, Spain
01/10/2019–30/11/2019
Interaction of molecules with nanoclusters supported on graphene.

Prof. Amand Lucas
University of Namur, Belgium
01/10/2019–31/10/2019
Surface physics.

Prof. Sergei Schemelinin
Weizmann Institute of Science, Rehovot, Israel
01/10/2019–Present
NEXT-SABAT

PhD student Michal Bialonczyk
Jagiellonian University, Kraków, Poland
01/11/2019–15/12/2019
Investigating full statistics of observables formed in a quantum phase transitions.

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

PhD student Efrem Bernuz Fitó
Universitat de Barcelona, Spain
11/11/2019–11/12/2019
Development of a software to calculate continuous measures of shape and symmetry.

Short visits

Prof. Juan Faustino Aguilera Granja
Instituto de Física de la Universidad Autónoma de San Luis Potosí, México
15/12/2018–04/01/2019
Óxidos metálicos bidimensionales.

PhD student Siddhartha Gurung Lopez
CEFCA, Centro de Física del Cosmos de Aragón, Teruel, Spain
06/01/2019–25/01/2019
Radiative transfer in star forming galaxies.

PhD student Daniele Spinoso
CEFCA, Centro de Física del Cosmos de Aragón, Teruel, Spain
06/01/2019–25/01/2019
Models of black hole formation.

Prof. Mateo Valero Cortes
Barcelona Supercomputing Center, Barcelona, Spain
10/01/2019–11/01/2019
Barcelona Supercomputing Center - past, present and future.

Prof. Josep María Martorell Rodon
Barcelona Supercomputing Center, Barcelona, Spain
11/01/2019–11/01/2019
Barcelona Supercomputing Center - past, present and future.

Prof. Lucía Aballe Aramburu
ALBA Synchrotron, Cerdanyola del Valles, Barcelona, Spain
14/01/2019–21/01/2019
Collaboration DIPC-ALBA.

PhD student Pau Besalú Sala
Universidad de Girona, Spain
14/01/2019–18/01/2019
Correct description of NLOP using DFT methods.

Prof. Josep Maria Luis Luis
Universidad de Girona, Spain
14/01/2019–18/01/2019
Design and application of new DFT functionals for the calculation of NLO properties.

Prof. Juan Ignacio Pérez Iglesias
Facultad de Ciencia Y Tecnologia, UPV/EHU, Leioa, Spain
18/01/2019–18/01/2019
Disarrangement of teenager brain.

Prof. Karolina Slowik
Institute of Physics, Nicolaus Copernicus University, Torun, Poland
18/01/2019–26/01/2019
Manipulating emission rates and interactions of quantum emitters beyond electric dipole approximation.

Dr. Vahagn Mkhitaryan
ICFO, Instituto de Ciencias Fotónicas, Casteldefels, Barcelona, Spain
20/01/2019–27/01/2019
Plasmonics with surface science quality devices.

Prof. Rolf Heid
Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany
21/01/2019–13/01/2019
Electronic and lattice dynamical properties of topological materials.

Prof. Angel Rivas Vargas
Facultad Ciencias Físicas, Universidad Complutense de Madrid, Spain
23/01/2019–26/01/2019
Open quantum systems.

Prof. Curt Wentrup
The University of Queensland, Australia
27/01/2019–29/01/2019
Experimental and computational studies of nitrenes, carbenes and diradicals.

Prof. Miguel Ángel Fernández Sanjuan
Universidad Rey Juan Carlos, Madrid, Spain
31/01/2019–02/02/2019
Nonlinear dynamics, chaos and complex systems: ahistorical perspective.

Prof. Antonio García Martín
IMN-CSIC, Madrid, Spain
04/02/2019–08/02/2019
Generalized couple-dipole methods.

PhD student Lucía Llópiz Domínguez
IMN-CSIC, Madrid, Spain
04/02/2019–01/03/2019
Generalized couple-dipole methods.

PhD student Diego Romero Abujetas
Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain
04/02/2019–13/02/2019
Theory of light scattering in nano-structured highly refractive media.

Dr. Geza Toth
University of the Basque Country, UPV/EHU, Donostia/San Sebastián, Spain
06/02/2019–06/02/2019
Entanglement between two spatially separated atomic modes.

Dr. Sahar Alipour
Aalto University, Espoo, Finland
10/02/2019–14/02/2019
Dynamics and thermodynamics and estimation in open quantum systems.

Dr. Ali Rezakhani
Sharif University of Technology, Tehran, Iran
10/02/2019–14/02/2019
Quantum information.

Uwe R. Fischer
Seoul National University, Seoul, South Korea
11/02/2019–22/02/2019
Discussions and Initiation of collaboration, oral presentation.

Eva M. Méndez Rodríguez
Universidad Carlos III de Madrid, Getafe, Spain
12/02/2019–13/02/2019
Open science from the inside out: concept, challenges and implementation.

Dr. Vahagn Mkhitaryan
ICFO, Instituto de Ciencias Fotónicas, Casteldefels, Barcelona, Spain
13/02/2019–14/02/2019
Plasmonics with surface science quality devices.

Dr. Zhida Song
Princeton University, New Jersey, USA
16/02/2019–01/03/2019
Topological band theory.

Prof. Iwo Bialynicki-Birula
Center for Theoretical Physics, Warsaw, Poland
17/02/2019–22/02/2019
Photon helicity in material media.

Prof. Antonio García Martín
Instituto de IMN-CSIC, Madrid, Spain
18/02/2019–22/02/2019
Generalized couple-dipole methods.

Prof. Kazutaka Takahashi
Tokyo Institute of Technology, Meguro, Tokyo, Japan
18/02/2019–02/03/2019
Shortcuts to adiabaticity.

Prof. David Nygren
University of Texas at Arlington, Texas, USA
19/02/2019–22/02/2019
Next / Sabat.

Prof. Jorge Dos Santos Pacheco
Universidade do Minho, Portugal
20/02/2019–22/02/2019
Evolutionary game theory of cooperation: from cells to societies.

Prof. Bogdan Andrei Bernevig
Princeton University, New Jersey, USA
22/02/2019–27/02/2019
Topological matter: classification and design.

Nicolas Regnault
Ecole Normale Superieure Paris -CNRS, París, France
22/02/2019–25/02/2019
Topological materials.

Dr. Mikel Sanz
QUTIS, UPV-EHU, Facultad de Química, Leioa, Spain
22/02/2019–22/02/2019
Digital-analog quantum computing: a paradigm for the NISQ era.

Prof. Salvador Miret Artes
CSIC, Instituto de Física Fundamental, Madrid, Spain
24/02/2019–01/03/2019
Electron phonon coupling.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
25/02/2019–06/03/2019
Surface electron-phonon interaction.

Dr. Kevin Vynck
LP2N (Laboratoire Photonique Numérique et Nanosciences), Institut d'Optique d'Aquitaine, Talence, France
26/02/2019–01/03/2019
Light propagation in disordered correlated media.

Dr. Thomas James Broadhurst
Ikerbasque, UPV/EHU, Leioa, Spain
27/02/2019–01/03/2019
New dark waves from the cosmos.

Prof. Carlos Hernández Monteagudo
CEFCA, Teruél, Spain
27/02/2019–02/03/2019
BACCO, cosmology.

Dr. Mark Neyrinck
UPV/EHU, Leioa, Spain
27/02/2019–28/02/2019
Constructing an optimally average universe.

Dr. Dmitri Efremov
Leibnitz Institute for Solid State Physics
and Material Science IFW, Dresden, Germany
01/03/2019–16/03/2019
Electronic excitations and superconducting
instability in solids.

Dr. Mikolaj Kajetan Schmidt
Macquarie University, Sydney, Australia
01/03/2019–17/03/2019
Cavity-quantum electrodynamics methods
for plasmon-enhanced molecular spectroscopy.

Dr. Linda A. Zotti
Universidad Autónoma de Madrid, Spain
05/03/2019–05/03/2019
Electronics based on biomolecules.

Prof. Humberto Bustince Sola
Universidad Pública de Navarra, Pamplona, Spain
09/03/2019–10/03/2019
Artificial intelligence.

Prof. Hua Guo
University of New Mexico, Albuquerque, USA
10/03/2019–16/03/2019
Adiabatic and non-adiabatic gas-surface
dynamics.

Prof. Claude Laurent Bonnet
Groupe THEO, ISM UMR5255, CNRS
Université de Bordeaux, France
11/03/2019–12/03/2019
Quantum effects gas-surface dynamics.

Prof. Pascal Larregaray
Groupe THEO, ISM UMR5255, CNRS
Université de Bordeaux, France
11/03/2019–12/03/2019
Recombination processes at surfaces.

Prof. Frank Pollmann
Technical University of Munich, Germany
11/03/2019–16/03/2019
Strong correlations.

PhD student Alberto Rodriguez Fernandez
Groupe THEO, ISM UMR5255,
CNRS/Université de Bordeaux, France
11/03/2019–12/03/2019
Quantum effects gas-surface dynamics.

Prof. Feliciano Giustino
Department of Materials,
University of Oxford, UK
19/03/2019–22/03/2019
Phonon-polarons and plasmon-polarons
in the ARPES spectra of transition metal oxides.

Prof. John Richard Bond
Canadian Institute for Theoretical Astrophysics,
University of Toronto, Canada
22/03/2019–26/03/2019
Scientific discussions on large scale structure
of the universe with raul angulo and silvia bonoli.

Dr. Pol Forn Díaz
Barcelona Supercomputing Center,
Barcelona, Spain
24/03/2019–26/03/2019
Quantum computing.

Prof. Didier Poilblanc
CNRS, Toulouse, France
24/03/2019–27/03/2019
Topological phases of matter
and tensor networks.

Prof. Valentyn Volkov
University of Southern Denmark (SDU)SDU
NanoOptics, The Mads Clausen Institute,
Odense, Denmark
24/03/2019–31/03/2019
Hybrid graphene-nanometallic structures.

PhD student Valentina Musumeci
Université de Bordeaux, France
25/03/2019–05/04/2019
Supercritical Fluids for cement based materials.

Prof. Dieter Richter
Forschungszentrum Jülich, Germany
25/03/2019–30/03/2019
Polymer dynamics.

Dr. Vahagn Mkhitaryan
ICFO, Instituto de Ciencias Fotónicas,
Casteldefels, Barcelona, Spain
26/03/2019–29/03/2019
Plasmonics with surface science quality devices.

Prof. Bjoern Malte Schafer
Zentrum fuer Astronomie der Universitatet
Heidelberg, Germany
26/03/2019–29/03/2019
Structure formation and gravitational lensing.

Prof. Paloma Adeva Ramos
Centro Nacional de Investigaciones Metalúrgicas
CSIC, Madrid, Spain
27/03/2019–28/03/2019
Metalurgia.

Dr. Ricardo Fernández
Centro Nacional de Investigaciones
Metalurgicas, CENIM, Madrid, Spain
28/03/2019–28/03/2019
A mesoscale approach to the creep
phenomenon.

Prof. Peter Feulner
Technical University of Munich, Germany
02/04/2019–06/04/2019
Photoemission studies of ultrafast electron
dynamics.

Prof. Guido Fratesi
Universitá di Milano, Italy
03/04/2019–06/04/2019
Theory of ultrafast charge-transfer at surfaces.

Prof. Juan Faustino Aguilera Granja
Instituto de Física, Universidad Autónoma
de San Luis Potosí, México
06/04/2019–30/04/2019
Propiedades electrónicas de nanosestructuras
y sistemas de baja dimensión.

Prof. Guy Le Lay
PIIM-CNRS, Aix-Marseille Université,
Marseille, France
07/04/2019–26/04/2019
Silicene.

Dr. Zakaria Abdelfattah
Faculty of Science, Al-Azhar University,
El Cairo, Egypt
10/04/2019–23/04/2019
Synchrotron radiation experiment.

Dr. Camila Correa
Leiden University, Netherlands
11/04/2019–12/04/2019
Topics of cosmology, dark matter
and galaxy formation.

Prof. Gregory D. Scholes
Princeton University, New Jersey, USA
11/04/2019–12/04/2019
Probing ultrafast chemical dynamics inspired
by the rhythms of pireflies.

Dr. Cesar Tomé López
Euskampus, Bilbao, Spain
11/04/2019–12/04/2019
The easiest hygienic chore: communicate your results to a broader audience.

Dr. Titouan Lazeyras
SISSA, Trieste, Italy
28/04/2019–03/05/2019
Large scale structure of the universe.

PhD student David Izquierdo Villalba
CEFCA, Centro de Física del Cosmos de Aragón, Teruel, Spain
29/04/2019–10/05/2019
Work on model of galaxy formation and black hole evolution.

Dr. Ignasi Pérez Ràfols
Laboratorire d'Astrophysique de Marseille (LAM), Marseille, France
29/04/2019–30/04/2019
Quasar selection methods.

PhD Student Daniele Spinoso
CEFCA, Centro de Física del Cosmos de Aragón, Teruel, Spain
29/04/2019–10/05/2019
Models of black hole formation.

Dr. Rolf Moeller
Fakultaet fuer Physik, Universitaet Duisburg-Essen, Germany
03/05/2019–04/05/2019
Following the steps of a chemical reaction or a 2D phase transition by scanning tunneling microscopy.

Dr. Paula Natalia Abufager
Instituto de Física Rosario, Rosario, Argentina
05/05/2019–01/06/2019
Electronic, magnetic and transport properties at the nanoscale.

PhD student Cliò Efthimia Agrapidis
Institute for Theoretical Solid State Physics, FW Dresden, Germany
05/05/2019–08/05/2019
Tensor networks and quantum many-body systems.

Prof. Shumpei Masuda
Tokyo Medical and Dental University, Japan
05/05/2019–11/05/2019
Control of quantum systems.

Prof. Christophe Rossel
IBM Research-Zurich, Rüschlikon, Switzerland
05/05/2019–19/05/2019
Cryogenic thermoelectric bolometer for broadband multipixel detectors.

Prof. Marcello Musso
ICTP-EAIFR, University of Rwanda - Kigali, Rwanda
08/05/2019–30/05/2019
Investigating analytical models of dark matter halos and testing their correspondence with analytic models.

Prof. Petra Rudolf
Zernike Institute for Advanced Materials, University of Groningen, Netherlands
09/05/2019–11/05/2019
Molecular motors and switches at surfaces.

Prof. Toru Hirahara
Tokyo Institute of Technology, Tokyo, Japan
12/05/2019–14/05/2019
Electronic structure of magnetic topological heterostructures.

Prof. George F. Smoot
University of California, and Lawrence Berkeley National Laboratory, Berkeley, USA
16/05/2019–17/05/2019
Gravitational waves, merging black holes and merging binary neutron stars.

Prof. Ignacio Iglesias Casarrubios
Universidad de Murcia, Murcia, Spain
20/05/2019–24/05/2019
Optical imaging.

Prof. David Abergel
Nature Physics, London, UK
22/05/2019–24/05/2019
Nature physics editor.

Dr. Vitaliy Goryashko
Uppsala University, Uppsala, Sweden
22/05/2019–01/06/2019
Nanoscale subsycle light sources.

Prof. Charles Lawrie
Biodonostia, Donostia/San Sebastián, Spain
23/05/2019–23/05/2019
Dark matter and liquid biopsies: molecular oncology research in Biodonostia.

Dr. Paul Weis
University of California, Los Angeles, USA
24/05/2019–24/05/2019
Atomically precise chemical, physical, and electronic nanoscale contacts.

Prof. Michel A. Van Hove
Hong Kong Baptist University, Hong Kong, China
25/05/2019–02/06/2019
Molecular Machines: Principles and Mechanisms.

Prof. Stephan Fritzsche
Helmholtz-Institut Jena, Jena, Germany
26/05/2019–31/05/2019
Photonics and plasmonics.

Prof. Yan Sun
Max Planck Institute for Chemical Physics of Solids, Dresden, Germany
27/05/2019–30/05/2019
Topological materials and transport.

Dr. José Flores Livas
University of Basel, Switzerland
28/05/2019–28/05/2019
In silico design of materials from quantum to exotic chemistry.

Dr. Catalin Gainaru
Technical Unversity of Dortmund, Germany
02/05/2019–31/05/2019
Dielectric spectroscopy and its relation to other experimental techniques.

Dr. Augustine Kshetrimayum
FU Berlín, Germany
01/06/2019–15/06/2019
Finite temperature algorithms for fermionic projected entangled pair states.

Dr. Alejandro Benítez Llambay
Institute for Computational Cosmology - Durham University, UK
02/06/2019–07/06/2019
Small scale structure in LCDM.

Prof. Mads Brandbyge
Technical University of Denmark, Denmark.
02/06/2019–07/06/2019
Electron transport in 2D materials.

Prof. Gilad Haran
Weizmann Institute of Science, Rehovot, Israel
02/06/2019–06/06/2019
Nanophotonics.

PhD student Luis Enrique Aguilar Suerez
Zernike Institute for Advanced Materials, Faculty of Science and Engineering, University of Groningen, Netherlands
03/06/2019–07/06/2019
Theoretical study of the singlet fission process.

Prof. Gustav Bihlmayer
Forschungszentrum Jülich, Germany
05/06/2019–08/06/2019
Exploring 2D magnetic topological materials by density functional theory.

PhD student José Aarón Rodríguez Jiménez
Instituto de Fisica Manuel Sandoval Vallarta, UASLP, San Luis Potosí, México
05/06/2019–08/06/2019
Quantum chemistry.

Prof. Alicia Sintes Olives
Universidad de les Illes Balears and LIGO, Palma de Mallorca, Spain
05/06/2019–06/06/2019
Hunt for gravitational waves.

Prof. Salvador Miret Artes
CSIC, Instituto de Física Fundamental, Madrid, Spain
08/06/2019–11/06/2019
Electron phonon coupling.

Dr. Hong-Hao Tu
Technical University of Dresden, Dresden, Germany
09/06/2019–14/06/2019
Exactly solvable quantum impurity model with inverse-square interactions.

Prof. Davide Donadio
University of California, Davis, USA
12/06/2019–20/06/2019
Vibrational and thermal properties of intercalated 2D materials.

Dr. Pramod P. Pillai
Indian Instiute of Science Education and Research (IISER) Pune, India
12/06/2019–13/06/2019
Regulation of interparticle interactions: in search of advanced nanoparticle functions.

Prof. Dave Nygren
University of Texas at Arlington, Texas, USA
13/06/2019–14/06/2019
The art of experiment and the pace of discovery in particle physics.

Dr. Oleksander Stetsovych
Technische Universität München, Czech Republic
13/06/2019–27/06/2019
Non-contact atomic force microscopy applied to on-surface synthesis.

Dr. Francisco Villaescusa Navarro
Flatiron Institute, New York, USA
13/06/2019–14/06/2019
Collaboration on large-scale structure.

Dr. Guillaume Hurier
CEFCA, Teruel, Spain
17/06/2019–21/06/2019
Study of the star formation history of galaxy cluster members.

Prof. Rémi Carminati
Institut Langevin, ESCPI, Paris, France
23/06/2019–29/06/2019
Light scattering.

Prof. John Schotland
University of Michigan, Ann Arbor, USA
23/06/2019–29/06/2019
Light scattering.

Dr. Hugo Dil
Ecole Polytechnique Fédérale de Lausanne, Switzerland
26/06/2019–28/06/2019
Spin-orbit phenomena in materials and quantum mechanics.

Prof. Gouchun Yang
Centre for Advanced Optoelectronic Functional Materials Research and Laboratory for UV Light-Emitting Materials and Technology of Ministry of Education, Northeast Normal University. Changchun, China
26/06/2019–07/07/2019
Pressure induced new materials: we will analyze new atomic structures of B-Na alloys under pressure, and characterize its physical properties.

PhD student Carmen Romo Luque
Universidad de Valencia, Valencia, Spain
02/07/2019–31/07/2019
PETALO a new concept of PET scanner.

Dr. Facundo Rodriguez
Instituto de Ciencias del Espacio, CSIC, Barcelona, Spain
03/07/2019–09/07/2019
Identification of galaxy groups in cosmological simulations.

Dr. Giandomenico Palumbo
Free University of Bruxelles, Belgium
08/07/2019–08/07/2019
Tensor Berry connections in topological phases of matter.

Dr. Philipp Wessels
University of Hamburg, The Hamburg Centre for Ultrafast Imaging (CUI), Germany
08/07/2019–11/07/2019
Ultracold and ultrafast: manipulating quantum gases with femtosecond laser pulses.

Dr. Zhida Song
Princeton University, New Jersey, USA
09/07/2019–17/07/2019
Topological band theory.

Prof. Benjamin Davidovitch
University of Massachusetts, Amherst, USA
10/07/2019–13/07/2019
Mechanics and patterns of graphene.

Prof. Alexander Golubov
University of Twente, Enschede, Netherlands
10/07/2019–16/07/2019
Topological superconductivity.

Prof. Bogdan Andrei Bernevig
Princeton University, New Jersey, USA
13/07/2019–17/07/2019
Topological magnetic materials.

Prof. Rodney D. Priestley
Pinceton University, New Jersey, USA
14/07/2019–28/07/2019
Glassy dynamics of polymers in confinement.

Prof. Pilar Coloma Escribano
IFIC, Valencia, Spain
15/07/2019–19/07/2019
Opportunities for neutrino physics using spallation sources.

Dr. Mark Neyrinck
Universidad del País Vasco, UPV/EHU, Leioa, Spain
15/07/2019–18/07/2019
Cosmological realizations and "Pangaussianization".

PhD student Federico Tosone
Università di Roma tor Vergata, Roma, Italy
15/07/2019–18/07/2019
Analytic models for galaxy clustering.

Dr. Luis Pedro García Pintos
University of Massachusetts, Boston, USA
15/07/2019–26/07/2019
Limits to perception in the quantum world.

Dr. Mario Galarreta
San Francisco, California, USA
18/07/2019–20/07/2019
Transferable skills program.

Prof. Nazim Mamedov
Institute of Physics, National Academy of Sciences, Baku Azerbayjan
21/07/2019–27/07/2019
Topological insulators.

PhD student Diego Romero Abujetas
Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain
22/07/2019–26/07/2019
Theory of light scattering in nano-structured highly refractive media.

Prof. Viktoriia Babicheva
College of Optical Sciences,The University of Arizona, Tucson, USA
27/07/2019–31/07/2019
All-dielectrics metasurfaces.

Prof. Jordi Miralda Escudé
Institut de Ciències del Cosmos, Universitat de Barcelona, Spain
28/07/2019–30/07/2019
Galaxy study at high redshift.

Dr. Pedro David García Fernández
Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Bellaterra, Barcelona, Spain
29/07/2019–19/07/2019
Photon-phonon interaction driven by complexity.

Dr. Maria Contel
Brooklyn College, The City University of New York, USA
08/08/2019–08/08/2019
Gold (I)-based compounds and their potential as chemo- and targeted- therapeutics for renal and breast cancer.

PhD student Ana Isabel Fernández-Tresguerres
Universidad de Oviedo, Asturias, Spain
26/08/2019–29/08/2019
Polaritons in biaxial crystals.

Dr. Vahagn Mkhitaryan
ICFO, Instituto de Ciencias Fotónicas, Casteldefels, Barcelona, Spain
26/08/2019–31/08/2019
Plasmonics with surface science quality devices.

PhD student Andreas Gebauer
Universitaet Bielefeld, Bielefeld, Germany
28/08/2019–06/09/2019
Time-resolved photoelectron spectroscopy.

Prof. Björn Trauzettel
Würzburg Univeristy, Würzburg, Germany
28/08/2019–04/09/2019
Topological superconductivity.

Prof. Javier Rodríguez Vázquez de Aldana
Universidad de Salamanca, Spain
08/09/2019–14/09/2019
Femtosecond direct inscription of 3D photonic structures in glass ceramic materials.

PhD student Georg Poelchen
IFMP, Dresden, Germany
09/09/2019–30/09/2019
Photoemission studies of 4f materials.

PhD student Susanne Schulz
TU, Technische Universität Dresden, Germany
16/09/2019–30/09/2019
Photoemission studies on 4f materials.

Prof. Gerhard Hummer
Max Planck Institute of Biophysics, Frankfurt, Germany
17/09/2019–20/09/2019
Unexpected complexities of macromolecular diffusion in membranes and dense protein solutions.

Prof. Bernardo Cervantes Sodi
Instituto de Radioastronomía y Astrofísica - Universidad Nacional Autónoma de México, Michoacán, México
18/09/2019–21/09/2019
Study of barred galaxies.

Prof. Francisco González Fernández
Facultad de Filosofía y Letras, Universidad de Oviedo, Spain
23/09/2019–24/09/2019
Creativum.

Prof. Juan Luis Suárez Sánchez de León
CulturePlex Lab at Western University, Ontario, Canada
23/09/2019–26/09/2019
Analyzing creativity with machine learning and big data.

Prof. Juan José Palacios Burgos
Universidad Autónoma de Madrid, Spain
26/09/2019–27/09/2019
Tales in 2D crystals.

PhD student Rishav Harsh
Université Paris-Diderot, Paris, France
30/09/2019–04/10/2019
Low temperature scanning tunneling microscopy and spectroscopy.

Dr. Luca Barbiero
Université libre de Bruxelles, Physics of Complex Systems (CENOLI), Bruxelles, Belgium
01/10/2019–04/10/2019
Engineering Z2 lattice gauge theories with a strongly atomic mixture.

Prof. Frank Pollmann
Technical University of Munich, Germany
07/10/2019–11/10/2019
Strong correlations.

Prof. Hadiseh Alaeian
University of Stuttgart, Stuttgart, Germany
09/10/2019–13/10/2019
Topological quantum photonics.

Dr. Janos Asbóth
Wigner Institute Budapest, Budapest, Hungary
10/10/2019–12/10/2019
Topological quantum optics.

Dr. Adán Cabello
Universidad de Sevilla, Spain
14/10/2019–15/10/2019
Quantum correlations: Where do their limits come from?

PhD student David Izquierdo Villalba
CEFCA, Centro de Física del Cosmos de Aragón, Teruel, Spain
14/10/2019–25/10/2019
Working in black hole growth and spin evolution.

PhD student Daniele Spinoso
CEFCA, Centro de Física del Cosmos de Aragón, Teruel, Spain
14/10/2019–25/10/2019
Modelling of BH formation at very redshift in the Lgalaxies semi-analytical model.

Prof. Priyamvada Natarajan
Yale University, New Haven, USA
16/10/2019–19/10/2019
Stress-testing the cold dark matter model with gravitational lensing.

Dr. Pablo Ares
National Graphene Institute, University of Manchester, UK
18/10/2019–18/10/2019
Scanning-probe-assisted nanowire circuitry.

Dr. Maxim Chernodub
Université de Tours, CNRS, France
21/10/2019–21/10/2019
Conformal anomaly in Dirac systems: transport, boundaries, and screening.

Prof. Giorgio Benedek
Università di Milano-Bicocca, Milano, Italy
25/10/2019–01/11/2019
Electron-phonon interaction at conducting surfaces; surface dynamics.

Prof. Kai Schmidt
Universitaet Erlangen, Nürengerg, Germany
26/10/2019–31/10/2019
Mutually attracting spin waves in the square-lattice quantum antiferromagnet.

Dr. Gustavo Bodelon
CINBIO-Universidad de Vigo, Spain
07/11/2019–08/11/2019
Bioinorganic chemistry to catalysis.

PhD student Philipp Schmoll
Johannes Gutenberg University of Mainz, Germany
17/11/2019–30/11/2019
Tensor networks for triangular lattices.

Prof. Eli Pollak
Weizmann Institute of Science, Rehovoth, Israel
23/11/2019–02/12/2019
Quantum backflow.

Prof. Salvador Miret Artés
Instituto de Física Fundamental, Madrid, Spain
24/11/2019–02/12/2019
Electron phonon coupling.

Prof. Didier Poilblanc
Université de Toulouse, CNRS, Toulouse, France
27/11/2019–29/11/2019
Tensor network approach to abelian and/or non-abelian topological spin liquids.

Dr. Liliana Arrachea
Universidad Nacional de San Martín, Buenos Aires, Argentina
08/12/2019–11/12/2019
Alternating currents through majorana bound states. Development of a floquet theory in the context of Bogolioubov-De-Gennes equations to treat spins on superconducting surfaces.

Prof. Akhlesh Lakhtakia
Pennsylvania State University, Pennsylvania, USA
08/12/2019–11/12/2019
Optoelectronic Optimization of Thin-Film Solar Cells

Prof. Pere Alemany i Cahner
Universitat de Barcelona, Barcelona, Spain
09/12/2019–13/12/2019
Development of a software to calculate continuous measures of shape and symmetry.

Prof. Miquel Llunell i Marí
Universitat de Barcelona, Barcelona, Spain
09/12/2019–13/12/2019
Development of a software to calculate continuous measures of shape and symmetry.

Dr. Kevin Vynck
LP2N (Laboratoire Photonique Numérique et Nanosciences), Institut d'Optique d'Aquitaine, Talence, France
09/12/2019–13/12/2019
Light propagation in disordered correlated media.

Dr. Itziar Aretxaga
Instituto Nacional de Astrofísica, Óptica y Electrónica, México
11/12/2019–11/12/2019
Dusty galaxies in formation 1-2 Gyrs after the Big Bang.

Prof. Peter Zoller
Institute for Quantum Optics and Quantum Information and University of Innsbruck, Austria
11/12/2019–13/12/2019
Quantum Optics.

Prof. Juan Faustino Aguilera Granja
Instituto de Física, Universidad Autónoma de San Luis Potosí, México
13/12/2019–Present
Low dimensional nanosystems and self assembled systems.

Personnel

Administration

Ana López de Goicoechea
Administrator
End of contract 30/06/2019

Olatz Leis
Director of Economics & Finance and Project Management

Beatriz Suescun
Director of Administration, Human Resources and Legal Area

Amaia Etxaburu
President's Assistant

María del Mar Álvarez
Administrative

Nerea Fariñas
Administrative

Karmela Alonso
Administrative

Natasha Nedashkivska
Administrative

Juan Burgos
Maintenance

Outreach

Nora González
Outreach Manager

Amaia Arregi
Outreach Officer

Peru Salaburu
Outreach Officer
End of contract 30/06/2019

Computing Center

Txomin Romero
Computing Center Director

Belén Isla
Computing Center Assistant Director and HPC Systems Manager

Carmen Martín
Systems, Security and Networks Manager

Luz Fernández
Operation and Help Desk Manager

Diego Lasa
Computing Services Manager

Daniel Franco
HPC Resources Technician

Urko Lekuona
Help Desk & Application Development Technician
End of contract 31/12/2019

Colloquia

1 Barcelona Supercomputing Center – past, present, and future
11/01/2019
Mateo Valero
Barcelona Supercomputing Center, Spain

2 Evolutionary Game Theory of Cooperation: From Cells to Societies
21/02/2019
Jorge M. Pacheco
Mathematics and Applications Department, University of Minho, Portugal

3 Molecular Motors and Switches at Surfaces
10/05/2019
Petra Rudolf
Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

4 Gravitational Waves, Merging Black Holes and Merging Binary Neutron Stars
16/05/2019
George F. Smoot
Physics Department and Lawrence Berkeley National Laboratory, University of California, Berkeley, USA
Institute for Advanced Study, Hong Kong University of Science and Technology, Hong Kong
Energetic Cosmos Laboratory, Nazarbayev University, Astana, Kazakhstan
Université Sorbonne Paris Cité, Université Paris Diderot, Paris, France

5 Hunt for gravitational waves
06/06/2019
Alicia Sintes
University of the Balearic Islands
LIGO Scientific collaboration

6 The art of experiment and the pace of discovery in particle physics
13/06/2019
David R. Nygren
University of Texas Arlington, USA
Lawrence Berkeley National Laboratory, University of California, Berkeley, USA

7 Unexpected complexities of macromolecular diffusion in membranes and dense protein solutions
19/09/2019
Gerhard Hummer
Max-Planck-Institut für Biophysik, Frankfurt, Germany

8 Stress-testing the cold dark matter model with gravitational lensing
17/10/2019
Priyamvada Natarajan
Departments of Astronomy and Physics, Yale University, USA

9 A Quantum Leap in Quantum Information – Building Quantum Computers and Quantum Simulators with Cold Atoms and Ions
12/12/2019
Peter Zoller
University of IQOQI of the Austrian Academy of Sciences, Innsbruck, Austria

Seminars

1 Large angle amplitude “spin strain waves”
17/01/2019
Lucia Aballe
ALBA Synchrotron, Cerdanyola del Valles, Barcelona, Spain

2 Disarrangement of teenager brain
18/01/2019
Juan Ignacio Perez
Facultad de Ciencia Y Tecnologia, UPV/EHU, Donostia/San Sebastián, Spain

3 Multiscale methods in solvated systems: from interfaces to biosensors
22/01/2019
Alexandre Reily Rocha
Insitute for Theoretical Physics, State University of São Paulo, Brazil

4 Manipulating emission rates and interactions of quantum emitters beyond electric dipole approximation
24/01/2019
Karolina Slowik
Nicolaus Copernicus University, Torun, Poland

5 Experimental and computational studies of nitrenes, carbenes and diradicals
28/01/2019
Curt Wentrup
The University of Queensland, Australia

6 Nonlinear dynamics, chaos and complex systems: a historical perspective
01/02/2019
Miguel A. Fernandez Sanjuan
Universidad Rey Juan Carlos, Madrid, Spain

7 Entanglement between two spatially separated atomic modes
06/02/2019
Geza Toth
University of the Basque Country, UPV/EHU, Donostia/San Sebastián, Spain

8 Thermodynamics of quantum systems in the presence of interaction and correlation
11/02/2019
Sahar Alipour
Aalto University, Espoo, Finland

9 Estimation in the quantum world
11/02/2019
Ali Rezakhani
Sharif University of Technology, Tehran, Iran

10 Open science from the inside out: concept, challenges and implementation
13/02/2019
Eva Mendez
Universidad Carlos III de Madrid, Getafe, Madrid, Spain

11 Twisted localized solutions of the dirac equation
20/02/2019
Iwo Bialynicki-Birula
Center for Theoretical Physics, Warsaw, Poland

12 Digital-analog quantum computing: a paradigm for the NISQ era
22/02/2019
Mikel Sanz
QUTIS, UPV-EHU Leioa, Spain

13 Electronics based on biomolecules
05/03/2019
Linda A. Zotti
Universidad Autónoma de Madrid, Madrid, Spain

14 Impurity effects in interaction driven topological insulators
07/03/2019
Dmitri Efremov
Leibnitz Institute for Solid State Physics and Material Science IFW, Dresden, Germany

15 Dynamics of surface reactions
15/03/2019
Hua Guo
University of New Mexico, Albuquerque, Mexico

16 Phonon-polarons and plasmon-polarons in the ARPES spectra of transition metal oxides
21/03/2019
Feliciano Giustino
University of Oxford, England

17 The quantum universe in the planck era and beyond (general public talk)
25/03/2019
Richard Bond
Canadian Institute for Theoretical Astrophysics, University of Toronto, Canada

18 Ultra-thin metal films for nanophotonics and optoelectronics
27/03/2019
Valentyn Volkov
University of Southern Denmark (SDU)SDU NanoOptics, The Mads Clausen Institute, Odense, Denmark

19 A mesoscale approach to the creep phenomenon
28/03/2019
Ricardo Fernández
Centro Nacional de Investigaciones Metalurgicas, CENIM, Madrid, Spain

20 Intrinsic alignments of galaxies in weak lensing
29/03/2019
Bjoern Malte Schaefer
Princeton University, New Jersey, USA

21 Helium physisorbed on metal surfaces and thorium layers on silver: zero-point motion and screening effects in photoemission and photoexcitation
03/04/2019
Peter Feulner
Technical University of Munich, Germany

22 Atom-thick oxides at the Fe(001) surface: from the playground for theory and experiments to applications
04/04/2019
Guido Fratesi
Universitá di Milano, Italy

23 Introduction to supermassive black holes
10/04/2019
Silvia Bonoli
DIPC, Donostia/San Sebastán, Spain

24 The easiest hygienic chore: communicate your results to a broader audience
11/04/2019
César Tomé
UPV/EHU-UPNA, Donostia/San Sebastián, Spain

25 Modelling galaxy formation in a cosmological context
12/04/2019
Camila Correa
Leiden University, Netherlands

26 Probing ultrafast chemical dynamics Inspired by the rhythms of fireflies
12/04/2019
Gregory D. Scholes
Princeton University, USA

27 Following the steps of a chemical reaction or a 2D phase transition by scanning tunneling microscopy
03/05/2019
Rolf Moeller
Fakultaet fuer Physik, Universitaet Duisburg-Essen, Germany

28 Coexistence of spontaneous symmetry breaking and topological order in the frustrated ferromagnetic J1-J2 chain
07/05/2019
Clio Efthimia Agrapidis
Institute for Theoretical Solid State Physics, FW Dresden, Germany

29 The technology challenges and progress for artificial intelligence
09/05/2019
Christophe Rossel
IBM Research-Zurich Laboratory, Switzerland

30 Unconscious bias: how it impacts careers in science and how to mitigate this influence
10/05/2019
Petra Rudolf
Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

31 Open science, open data, how much do you care?
17/05/2019
Christophe Rossel
IBM Research-Zurich Laboratory, Switzerland

32 Dark matter and liquid biopsies: molecular oncology research in Biodonostia
23/05/2019
Charles Lawrie
Biodonostia, Donostia/San Sebastián, Spain

33 Atomically precise chemical, physical, and electronic nanoscale contacts
24/05/2019
Paul Weiss
University of California, Los Angeles, USA

34 In silico design of materials from quantum to exotic chemistry
28/05/2019
José Flores-Livas
University of Basel, Switzerland

35 Attosecond free-electron lasers
29/05/2019
Vitaliy Goryashko
Uppsala University, Sweden

36 Linear and second order responses in topological semimetals
29/05/2019
Yan Sun
Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

37 Excursion sets, peaks and other creatures: improved analytical models of large scale structure
30/05/2019
Marcello Musso
EAIFR, Rwanda

38 Excitation and ionization of atoms by twisted light
30/05/2019
Stephan Fritzsche
Helmholtz-Institut Jena, Germany

39 Dielectric spectroscopy and its relation to other experimental techniques
30/05/2019
Catalin Gainaru
Technische Universität Dortmund, Germany

40 Molecular machines: principles and mechanisms
31/05/2019
Michel A. Van Hove
Hong Kong Baptist University, Hong Kong, China

41 Single-particle chemical physics: from plasmonic strong coupling to microsecond motions in biological machines
03/06/2019
Gilad Haran
Weizmann Institute of Science, Rehovot, Israel

42 Exploring 2D magnetic topological materials by density functional theory
06/06/2019
Gustav Bihlmayer
Forschungszentrum Jülich, Germany

43 Exactly solvable quantum impurity model with inverse-square interactions
11/06/2019
Hong-Hao Tu
TU Dresden, Germany

44 Tensor network investigation of the double layer kagome compound Ca_10Cr_7O_28
11/06/2019
Augustine Kshetrimayum
FU Berlin, Germany

45 Regulation of interparticle interactions: in search of advanced nanoparticle functions
13/06/2019
Pramod P. Pillai
Indian Instiute of Science Education and Research (IISER) Pune, India

46 Nanophononic devices from intercalated 2D materials
18/06/2019
Davide Donadio
University of California Davis, USA

47 Spin-orbit phenomena in materials and quantum mechanics
27/06/2019
Hugo Dil
Ecole Polytechnique Fédérale de Lausanne, Switzerland

48 Tensor berry connections in topological phases of matter
08/07/2019
Giandomenico Palumbo
Free University of Bruxelles, Belgium

49 Ultracold and ultrafast: manipulating quantum gases with femtosecond laser pulses
10/07/2019
Philipp Wessels
University of Hamburg, Germany

50 Computational enzymology: a comprehensive approach to study diverse mechanisms of RNA catalysis
11/07/2019
Darrin M. York
Rutgers University, New Jersey, USA

51 Novel 2D electron systems at the surface of functional oxides
16/07/2019
Andres Santander-Syro
Université Paris-Sud, France

52 Electronic structure of the hidden-order transition in URu2Si2
17/07/2019
Andres Santander-Syro
Université Paris-Sud, France

53 Opportunities for neutrino physics using spallation sources
18/07/2019
Pilar Coloma
IFIC, Valencia, Spain

54 Photon-phonon interaction driven by complexity
29/07/2019
Pedro David Garcia
Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, Barcelona, Spain

55 Novel material platforms and transdimensional lattices for metaphotonic devices
30/07/2019
Viktoriia Babicheva
University of Arizona, Tucson, USA

56 Gold (I)-based compounds and their potential as chemo- and targeted- therapeutics for renal and breast cancer
08/08/2019
Maria Contel
Brooklyn College, The City University of New York, USA

57 Chirality Josephson current due to a novel quantum anomaly in Weyl semimetals
03/09/2019
Björn Trauzettel
Würzburg University, Germany

58 A time-dependent approach to vibrational and vibronic spectroscopy: from molecules to surfaces
20/09/2019
Peter Saalfrank
University of Potsdam, Germany

59 Tales in 2D crystals
27/09/2019
Juanjo Palacios
Universidad Autónoma de Madrid, Spain

60 Engineering Z2 lattice gauge theories with a strongly interacting atomic mixture
02/10/2019
Luca Barbiero
Université Libre de Bruxelles, Belgium

61 Hybrid atomic-photonics: new paradigm for integrated quantum optics
10/10/2019
Hadiseh Alaeian
Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring, Stuttgart, Germany

62 Topological phases of quantum walks and how they can be detected
11/10/2019
Janos Asboth
Wigner Research Centre for Physics, and Budapest University of Technology and Economics, Hungary

63 Quantum correlations: where do their limits come from?
14/10/2019
Adán Cabello
Universidad de Sevilla, Spain

64 Scanning-probe-assisted nanowire circuitry
18/10/2019
Pablo Ares
Department of Physics and Astronomy & National Graphene Institute, University of Manchester, UK

65 Conformal anomaly in Dirac systems: transport, boundaries, and screening
21/10/2019
Maxim Chernodub
University of Tours, CNRS, France

66 Mutually attracting spin waves in the square-lattice quantum antiferromagnet
28/10/2019
Kai Schmidt
University of Erlangen, Germany

67 Lower bounds to eigenvalues
28/11/2019
Eli Pollak
Weizmann Institute of Science, Israel

68 Direct and inverse hall effects: a consequence of both Ampere's law and electron spin?
05/12/2019
Antonio Hernando
Universidad Complutense Madrid, Spain

69 Optoelectronic optimization of thin-film solar cells
09/12/2019
Akhlesh Lakhtakia
Pennsylvania State University, USA

70 Heat to work conversion in the quantum spin hall effect
10/12/2019
Liliana Arrachea
Universidad Nacional de San Martín, Argentina

71 Dusty galaxies in formation 1-2 Gyrs after the Big Bang
11/12/2019
Itziar Aretxaga
Instituto Nacional de Astrofísica, Óptica y Electrónica, Tonantzintla, México

Workshops

Engineering Quantum Open Systems

February 12, 2019
UPV/EHU, Leioa
https://aureliachenu.wixsite.com/eqos2019

Organizing Committee
Aurelia Chenu (Ikerbasque, DIPC)
Adolfo del Campo (Ikerbasque, DIPC)
Inigo Egusquiza (UPV/EHU)

This one-day workshop gathered invited and local experts on dynamics of open quantum systems.

Invited Speakers
Sahar Alipour (Aalto University)
Aurelia Chenu (DIPC)
Adolfo del Campo (DIPC)
Uwe Fischer (Seoul National University)
Geza Giedke (DIPC)
Ali Rezakhani (Sharif University)
Geza Toth (UPV/EHU)
Lian-Ao Wu (UPV/EHU)

3S'19 Symposium on Surface Science

March 10-16, 2019
Hotel Tuc Blanc, Baqueira Beret
http://dipc.ehu.es/3s19/

Organizing Committee
Daniel Sanchez Portal (CFM-CSIC, DIPC)
Enrique Ortega (CFM-UPV/EHU, DIPC)
Andres Arnau (CFM-UPV/EHU, DIPC)
Pedro Echenique (CFM-UPV/EHU, DIPC)

Since its foundation in 1983, the 3S Symposium on Surface Science as a winter school by members of the Institut für Allgemeine Physik (renamed recently to Institute of Applied Physics) of the Vienna University of Technology (TU Wien), its format has been kept following the spirit of the Gordon Conferences. This means that there is ample time for discussions and joint outdoor activities for the participants. The attendance of the symposium was kept below 100 participants so that active communication between all members could be guaranteed.

The conference seeks to promote the growth of scientific knowledge and its effective exchange among scientists in the field of surface physics and related areas, including applied topics. In this 32nd edition, the program has focused on multilayered nanostructures and low dimensional systems, including fundamental aspects and their applications. A large variety of prestigious experimental and theoretical researchers has contributed to the success of the Symposium.

DIPC Symposium on Quantum Science

March 26, 2019
DIPC, Donostia/San Sebastián
http://dipc.ehu.es/ws_presentacion.php?id=204

Organizing Committee
Román Orús (DIPC, Ikerbasque)

In this one-day symposium we discussed about topics related to strongly correlated systems, tensor network states and methods, and quantum technologies. We had a combination of theoretical and experimental talks, together with in-depth discussions on some topics.

Invited Speakers
Saeed Jahromi (DIPC)
Didier Poilblanc (Université de Toulouse, CNRS)
Pol Forn (BSC)
Maia Garcia-Vergniory (DIPC, Ikerbasque)
Adolfo del Campo (DIPC, Ikerbasque)

3rd Basque Quantum Science and Technology Workshop

May 23, 2019
Lecture Hall, CIC nanoGUNE, Donostia/San Sebastián
http://dipc.ehu.es/giedke/eusqutech19.html

Organizing Committee
Dario Bercioux (DIPC, Ikerbasque)
Adolfo del Campo (DIPC, Ikerbasque)
Géza Giedke (DIPC, Ikerbasque)
Lucas Lamata (UPV/EHU)
Roman Orús (DIPC, Ikerbasque)
Enrique Rico (UPV/EHU, Ikerbasque)
Enrique Solano (UPV/EHU, Ikerbasque)

The meeting continues a series started in 2015. It aims to bring together the growing community of researchers working on quantum science and technology and related fields in the Basque Country and to nurture and facilitate interaction, discussion, and collaboration between them. Since the last workshop, several colleagues with a focus on quantum science joined our community and several of them had the opportunity to present their work at this workshop.

The workshop attracted between 30 and 40 participants, about half of them PhD students. Animated discussions in the concluding poster session (with about 15 posters) concluded the event. The series will be continued next year in Bilbao.

Invited Speakers
Gabriel Molina-Terriza (CFM, Ikerbasque)
Adolfo del Campo (DIPC, Ikerbasque)
Lucas Lamata (UPV/EHU)
David Abergel (NatureSpringer)
José Ignacio Pascual (nanoGUNE, Ikerbasque)
Aurelia Chenu (DIPC, Ikerbasque)
Roman Orús (DIPC, Ikerbasque)

Symposium S05 on "Nanoscience of colloids, molecular materials and polymers for sustainable society" at XXXVII Biennial Meeting of RSEQ

May 27, 2019
Kursaal, Donostia/San Sebastián
http://bienal2019.com/

Organizing Committee
Julio San Román del Barrio (ICTP-CSIC, Madrid)
Marek Grzelczak (DIPC, Donostia/San Sebastián)

The aim of the symposium was to provide a forum for the scientific community to exchange the knowledge and stimulate a crosstalk between research areas that are related to molecular nanomaterials, polymers, and colloidal systems. We have hosted 42 contributions (7 invited talks, 8 oral communications, 6 flash communications, 26 posters) of original research that addressed the aspect of the synthesis, advanced characterization and theoretical analysis of nanomaterials ranging from molecular and polymer to colloidal length-scales. Therefore, we have promoted the exchange the knowledge on the applications of emergent materials and sustainable chemical processes in the environmental, health and energy-related sectors.

Invited Speakers
Thuc-Quyen Nguyen (University of California)
Tomás Torres (Universidad Autónoma de Madrid, Spain)
Markus Antonietti (Max Planck Institute of Colloids and Interfaces, Potsdam, Germany)
Prashant V. Kamat (University of Notre Dame, USA)
Andreas Walther (Albert Ludwigs Universität Freiburg, Germany)
Paul S. Weiss (University of California, Los Angeles, USA)
Marcelo Calderón (POLYMAT, Donostia/San Sebastián, Spain)

Symposium S06 on "Synergies between computational and experimental chemistry" at XXXVII Biennial Meeting of RSEQ

May 27, 2019
Kursaal, Donostia/San Sebastián
http://bienal2019.com/

Organizing Committee
Jesus M. Ugalde (UPV/EHU, Donostia/San Sebastián, Spain)
Iñaki Tuñón (Universidad de Valencia, Spain)

Computational chemistry is a well-established discipline that has a fundamental role nowadays in the development, study and optimization of many chemical, physical and biological processes. The use of theoretical and computational models for the study of the properties of new materials, reaction mechanisms of catalytic reactions and in processes related to the chemistry of life, is nowadays a useful and transverse tool in many areas of chemical science. In this symposium we will focus on different relevant and state-of-the-art aspects of applied computational chemistry. One session will be devoted to each of the following fields:

- Frontiers in Molecular Structure Theory.
- Reaction Mechanisms & Catalysis.
- Materials Chemistry & Design.
- Computational Biochemistry.
- Excited State Chemistry.

Topics included:
- Quantum Chemical Modeling of Mechanisms and Selectivities in Homogeneous Catalysis.
- Synergy between theory, simulation and experiment for single-molecule protein folding.
- Developing and Benchmarking New DFT Methods for Challenging Chemical Systems.
- Absorption of low energy UV radiation by DNA: excited states and reactivity.
- Chemically active domains of liquids.

Invited Speakers
Fahmi Himo (Stockholm University, Sweden)
David de Sancho (EHU/UPV, DIPC, Spain)
Juan-Carlos Sancho-García (Universidad de Alicante, Spain)
Dimitra Markovitsi (Université Paris-Saclay, CNRS, France)
Barbara Kirchner (Universität Bonn, Germany)

Theoretical Chemistry and Computational Modeling: 20 years promoting Excellence in Science

May 30-June 1, 2019
DIPC, Donostia/San Sebastián
http://tccm2019.dipc.org

Organizing Committee
Jose M. Mercero (UPV/EHU, DIPC)
Xabier Lopez (UPV/EHU, DIPC)
Cedric Crespo (Bordeaux Université)
Manuel Alcami (Universidad Autónoma de Madrid)
Andoni Ugartemendia (UPV/EHU)
David Silva (UPV/EHU)
Oksana Azpitarte (UPV/EHU)

Scientific Committee
Jesus M. Ugalde (UPV/EHU, DIPC)
Cedric Crespo (Bordeaux Université)
Manuel Yañez (Universidad Autónoma de Madrid)
Darrin M. York (Rutgers University)

The Theoretical Chemistry and Computational Modeling: 20 years promoting excellence in science symposia has as an objective to get together European scientists of the theoretical chemistry area that have been involved on the homonymous Master that is celebrating the 20th anniversary.

Invited Speakers
Daniel Roca (ICMOL/UV)
Alicia Palacios (Universidad Autónoma de Madrid)
Ferran Freixas (IQCC/UdG)
Julia Contreras (University of Pittsburgh Medical Center)
Lola Gonzalez (Universidad de Salamanca)
Eduard Matito (DIPC, Ikerbasque)
Jose Javier Ruiz Pernia (Universidad de Valencia)
Maria Besora (Universidad Rovira i Virgili)
Sergio Martí (Universitat Jaume I)

Quantum Designer Physics

July 1-4, 2019
Miramar Palace, Donostia/San Sebastián
http://qdp2019.dipc.org/

Organizing Committee
Daniel Loss (University of Basel)
Francisco Guinea (University of Manchester)
Andres Arnau (CFM-UPV/EHU, DIPC)
Vitaly Golovach (CFM-UPV/EHU, DIPC, Ikerbasque)

The workshop was organized with the aim to introduce the concept of Quantum Design in the community of Condensed Matter Physics. As a result, Quantum Designer Physics was born during this workshop as a synergy between several most active fields in Condensed Matter Physics related in one way or another to quantum technologies and all focused on exploring the quantum properties of matter at the nanoscale with the purpose of designing new systems aimed to exhibit remarkable quantum behaviors and quantum functionalities. The workshop highlighted recent advances in quantum materials, topological states of matter, Majorana fermions, exotic superconducting hybrid systems, quantum magnetism, spintronics, and quantum computing.

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 n-dimensional materials. We updated on the progress in spin-based quantum computing with a look into the prominent future of quantum technologies. The quest for Majorana bound states in hybrid superconducting systems and topological quantum computing were also thoroughly discussed. Thus, we brought together the leading experts in almost all most advanced quantum technologies and created a stimulating atmosphere for discussing new quantum physics on the marvelous sites of San Sebastián. The workshop was filled with a sense of unity around the idea of everyone being a quantum designer, which has definitely fostered collaborations and has inspired the attendants to tackle new problems in fundamental physics, work on applications, and advance the futuristic technologies to become soon a reality. The worksop was also a great opportunity for the younger participants to learn and get started with great ideas in one of these quickly developing fields at the outermost frontier of Nanoscience.

Invited Speakers
Ramon Aguado (ICMM, CSIC, Madrid)
Javier Aizpurua (CFM-CSIC, Donostia)
Sebastian Bergeret (CFM-CSIC, Donostia)
Deungjang Choi (CFM, Donostia)
Evgueni Chulkov (CFM-EHU, DIPC, Donostia)
Klaus Ensslin (ETH, Zürich)
Akira Furusaki (RIKEN)
Jelena Klinovaja (University of Basel)
Roman Lutchyn (MS StationQ, Santa Barbara)
Hector Ochoa (Columbia University)
Yuval Oreg (Weizmann Institute)
Enrique Ortega (CFM-EHU, Donostia)
Gloria Platero (ICMM, CSIC, Madrid)
Daniel Rodan-Legrain (MIT)
Patrik Recher (TU Braunschweig)
Constantin Schrade (MIT)
Christian Schönenberger (University of Basel)
Jairo Sinova (Johannes Gutenberg University Mainz)
Hadar Steinberg (Hebrew University, Jerusalem)
Björn Trauzettel (Universität Würzburg)
Maria Vozmediano (ICMM, CSIC, Madrid)
Niels Walet (University of Manchester)
Richard Warburton (University of Basel)
Roland Wiesendanger (University of Hamburg)
Dominik Zumbühl (University of Basel)

Quantum Simulation: Gauge Fields, Holography, and Topology

July 10-12, 2019
Grade meeting room, Campus Leioa, UPV/EHU, Bilbao, Spain
https://sites.google.com/view/quant-sim-ght

Organizing Committee
E. Rico (UPV/EHU, Ikerbasque)
M.G. Vergniory (DIPC, Ikerbasque)

Scientific committee
G.K. Brennen (Macquarie Univ, Sydney)
A. Del Campo (DIPC, Ikerbasque)
S. Montangero (Università di Padova)

During the last years, a synergy among different fields in physics has grown up to understand and characterize, to control and manipulate quantum many-body systems that appear in high-energy physics and condensed matter models. Thanks to this collaborative effort, new tools and concepts from quantum information and quantum optics complement more traditional ones from particle and statistical physics.

The purpose of this workshop is to bring together in a three days meeting, experts and leaders in the field to present and discuss the most recent results and outlook the most promising directions of this multidisciplinary challenge.

Invited Speakers
M. Aidelsburger (LMU, Munich)
M.C. Bañuls (MPQ, Munich)
A. Bermudez (Universidad Complutense, Madrid)
B.A. Bernevig (Princeton University)
H. Bombin (Yukawa ITP)
M. Dalmonte (SISSA & ICTP, Trieste)
A. Dauphin (ICFO, Barcelona)
G. De las Cuevas (Universität Innsbruck)
J. Eisert (Freie Universität, Berlin)
L. Fallani (LENS, Florence)
P. Hauke (Universität Heidelberg)
S. Iblisdir (Universidad de Barcelona)
F. Jendrzejewski (Universität Heidelberg)
C. Kokail (IQOQI, Universität Innsbruck)
S. Kostka (NSC, Poland)
M.A. Martín-Delgado (UCM)
K. Meichanetzidis (Oxford University)
A. Miyake (University of New Mexico)
T. Neupert (Universität Zurich)
J. Pachos (University of Leeds)
F. Pollmann (TUM, Munich)
N. Regnault (ENS Paris)
M. Ringbauer (Universität Innsbruck)
S. Singh (Max-Planck Institute, Potsdam)
T. Stace (University of Queensland, Brisbane)
F. Verstraete (Ghent, University of Vienna)

Science of Cement and Related Complex Materials

July 15-18, 2019
Miramar Palace, Donostia/San Sebastián
http://scrcm19.dipc.org/

Organizing Committee
Andres Ayuela (CSIC-UPV/EHU-MPC, DIPC)
Jorge S. Dolado (CSIC-UPV/EHU-MPC, DIPC)
Silvina Cerveny (CSIC-UPV/EHU-MPC, DIPC)
Juan José Gaitero (TECNALIA R&I)
Edurne Erkizia (TECNALIA R&I)
Jose Ramón Leiza (Polymat, UPV/EHU)
Hegoi Manzano (UPV/EHU)

The workshop aims to bring together physicists, chemists, material scientists, and engineers to share their latest findings in the computational and experimental characterization of complex materials in general, but paying special focus on cementitious materials and their bewildering phenomena. Furthermore, it aims to integrate science and technology of complex materials such as cements. Participants would share their latest results in a comprehensive format related to the future opportunities of these materials.

Topics included:
- Clinkering. Crystalline phases.
- Hydration processes.
- Formation and growth of C-S-H gel. Mechanical and volume properties.
- Performance and characterization. Durability and sustainability of concrete.
- Composites based on cement. Nano additions and nano-reinforcements.
- Non-portland types of cement.
- Industrial application ideas.

Invited Speakers
Eng. Ippei Maruyama (Graduate School of Environmental Studies, Nagoya University, Japan)
Patrick Juilland (Construction Materials, Sika Technology AG, Switzerland)
Torben Gaedt (BASF Construction Solutions GmbH, Trostberg, Germany)
Päivö Kinnunen (University of Oulu, Finland)
Romain Dupuis (MIT, USA)
Guang Ye (TU Delft, The Netherlands)
Gaurav N. Sant (University of California, UCLA, USA)
Eduardus Koenders (TU Darmstad, Germany)
Faustino Aguilera Granja (Universidad de San Luis Potosi, Mexico)

Designing artificial quantum matter

July 15-19, 2019
Miramar Palace, Donostia/San Sebastián
http://daqm.dipc.org

Organizing Committee
Dario Bercioux (DIPC, Donostia/San Sebastián)
Reyes Calvo (CIC-Nanogune, Donostia/San Sebastián)
Geza Giedke (DIPC, Donostia/San Sebastián)
Nathan Goldman (Université libre de Bruxelles)
Matteo Rizzi (University of Cologne & Forschungszentrum Jülich)
Ingmar Swart (Utrecht University)

This multidisciplinary workshop aims to gather experts on different approaches to analog quantum simulations and foment interaction and discussion between the different communities. Keynote lectures will cover approaches based on:
- Cold atoms.
- Trapped ions.
- Photons.
- Electrons in engineered potentials.
- Superconducting circuits.

Topics included:
- Synthetic topological Floquet quantum matter.
- From Quantum Magnetism to Quantum Chemistry - New Avenues for Ultracold Quantum Gases.
- Quantum fluids of light in semiconductor microcavities.
- A step for gauge fields in lattices and a twist by dissipation.
- Controlling Many-Body States of Light.
- Electron quantum simulators: an experimental point of view.
- There is plenty of room at the bottom, the physics of electron quantum simulators.
- New Frontiers on Many-body Physics with Atomic Clocks.
- Experimental Quantum Simulations in "Artificial" Arrays of Trapped Ions (and Atoms).
- Making Quantum Matter from Light.

Invited Speakers
Alexander Altland (University of Cologne)
Immanuel Bloch (MPQ, Garching, Germany)
Jacqueline Bloch (C2N, Paris, France)
Tilman Esslinger (ETH Zürich, Switzerland)
Steve Girvin (Yale University, New Haven USA)
Hari C. Manoharan (Stanford University, Palo Alto USA)
Cristiane Morais Smith (Utrecht University, Utrecht, The Netherland)
Ana Maria Rey (JILA, NIST and University of Colorado, Boulder, USA)
Tobias Schätz (Albert-Ludwigs Universität, Freiburg, Germany)
Jonathan Simon (University of Chicago, Chicago, USA)

Silicon quantum electronics workshop 2019

October 14-16, 2019
Ignacio María Barriola Building, Donostia/San Sebastián
http://siqew2019.dipc.org/

Organizing Committee
María José Calderón (Instituto de Ciencia de Materiales de Madrid, CSIC)
Fernando González-Zalba (Hitachi Laboratory Cambridge)
Rubén Ochoa (DIPC and Hitachi Laboratory Cambridge)
Gloria Platero (Instituto de Ciencia de Materiales de Madrid, CSIC)
José Carlos Abadillo-Uriel (University of Wisconsin-Madison)

The Silicon Quantum Electronics Workshop is the annual meeting for the international community working on silicon-based approaches to realizing quantum electronics circuitry such as quantum computers. In this occasion, more than 200 people attended the three days of the workshop.

Topics included:
- Qubit implementations in silicon, silicon-germanium and germanium.
- Advances in materials and fabrication.
- Cryogenic classical (nano)-electronics and classical electronic interfaces with qubits.
- Computer-assisted design and analysis of dopant and quantum dot architectures.
- Theory and modeling of charge and spin decoherence mechanisms in silicon.
- Quantum error correction.
- Approaches to multi-qubit and coherent on-chip communication.
- Hybrid-qubit approaches combining Si and/or SiGe with other qubit systems.

Invited Speakers
This workshop is the 2019 edition of a series of workshops on silicon quantum electronics that have taken place roughly once a year since 2007. In keeping with the tradition that has developed, there are no invited speakers. There were 51 contributed talks representing the activities of basically all the groups in the world working on this topic.

Quantum Speed Limits and Thermodynamics

October 28-31, 2019
Grade meeting room, Campus Leioa, UPV/EHU, Bilbao, Spain
http://dipc.ehu.es/QSLThermo19

Organizing Committee
Aurelia Chenu (Ikerbasque, DIPC)
Fernando Gomez-Ruis (DIPC)
Adolfo del Campo (Ikerbasque, DIPC)
Lucas Celeri (UPV/EHU)
Inigo Egusquiza (UPV/EHU)

The international meeting "Quantum Speed limits and Thermodynamics" gathered world-wide leading experts on quantum science and technology working at the interface of quantum control, far-from-equilibrium physics, and quantum information science. Quantum speed limits are a set of fundamental results in information geometry that provide bounds on the rate at which physical processes can occur, the limits of computational power of physical devices, and the performance of quantum machines. The engineering of energy-efficient thermal machines and the optimization of quantum processes, including information processing, are at the forefront of quantum thermodynamics, which describes the thermodynamics of small quantum systems. The interplay of these two topics is currently a fast-paced area of research and the focus of the meeting. The workshop created a stimulating environment with a high level of presentations, providing the floor for rich discussions. Time allowed for discussions enabled the participants to deepen their particular interest, and invited for new collaborations. All participants were extremely happy with the events and congratulated the organizers.

Invited Speakers
Sahar Alipour (Aalto University, Finland)
Daniel Alonso (Universidad de la Laguna, Spain)
Steve Campbell (University College Dublin, Ireland)
Ines de Vega (Ludwid-Maximilians Universität Munchen, Germany)
Luis Pedro Garcia-Pintos (University of Maryland, USA)
John Goold (Trinity College Dublin, Ireland)
Matteo Lostaglio (ICFO, Spain)
Ahsan Nazir (The University of Manchester, UK)
Norman Margolus (MIT, USA)
Kavan Modi (Monash University, Australia)
Javier Molina-Vilaplana (Universidad Politecnica de Cartagena, Spain)
Mauro Paternostro (Queen's University Belfast)
Ali Rezakhani (Sharif University of Technology, Iran)
Angel Rivas (Universidad Complutense de Madrid)
Lukas Rudniki (Center for theoretical Physics PAS, Poland)
Kazutaka Takahashi (Tokyo Institute of Technology, Japan)
Zhen-Yu Xu (Soochow University, China)
Xi Chen (UPV/EHU)
Mikel Sanz (UPV/EHU)
Geza Toth (UPV/EHU)

DIPC-MIPT workshop

November 6-7, 2019
DIPC, Donostia/San Sebastián
http://dipc-mipt-2019.dipc.org

Organizing Committee
Alexey Nikitin (DIPC, Ikerbasque, Spain)
Valentyn Volkov (MIPT, Russia)

The workshop has been the starting point for the close collaboration between Donostia International Physics Center and Moscow Institute of Physics and Technology. The research lines relevant for both centers have been presented.

Invited Speakers
Ricardo Díez Muiño (DIPC)
Alexey Nikitin (DIPC)
Aitzol Garcia Etxarri (DIPC)
Daniel Sánchez-Portal (DIPC)
Aran Garcia-Lekue (DIPC)
David Casanova (DIPC)
Eugene Chulkov (DIPC)
Fabienne Barroso Bujans (DIPC)
Javier Aizpurua (DIPC)
Juanjo Saenz (DIPC)
Maia Garcia Vergniory (DIPC)
Marek Grzelczak (DIPC)
Paola Ferrario (DIPC)
Roman Orus (DIPC)
Yurii Rakovich (DIPC)
Valentyn Volkov (MIPT)
Andrey Vyshnevy (MIPT)
Boris Gorshunov (MIPT)
Dmitri Chubich (MIPT)
Dmitri Ponomarev (MIPT)
Dmitrii Svintsov (MIPT)
Dmitry Filonov (MIPT)
Sergei Novikov (MIPT)
Sergey Filippov (MIPT)
Nikita Orekhov (MIPT)
Tagir Aushev (MIPT)

From Bioinorganic Chemistry To Catalysis

November 8,2019
Faculty of Chemistry, UPV/EHU Donostia/San Sebastián
http://dipc.ehu.eus/ws_presentacion.php?id=213

Organizing Committee
Zoraida Freixa (Ikerbasque, UPV/EHU, Spain)
Luca Salassa (Ikerbasque, DIPC, Spain)
Miguel Huertos (Ikerbasque, UPV/EHU, Spain)
Jon M. Matxain (UPV/EHU, DIPC, Spain)
Eider San Sebastián (UPV/EHU, Spain)
Alessio Terenzi (DIPC, Spain)
Marek Grzelczak (Ikerbasque, CIC biomaGUNE, Spain)

This one-day workshop brought together researchers active in the interconnected fields of molecular catalysis and bioinorganic chemistry, targeting an audience of young master and doctorate students. The aim of the meeting was to create new synergies among researchers working in various research institutes located in Donostia. The workshop also counted with the kind participation of Dr. Gustavo Bodelón González (Colloid Chemistry Group of the University of Vigo).

Invited Speakers
Gustavo Bodelón González (University of Vigo)
Aitziber Cortajarena (CIC biomaGUNE)
Monica Carril (Biofisika)
J. Luis Delgado (Polymat and UPV/EHU)
Carlos Sanchez Cano (CIC biomaGUNE)
Eider San Sebastián (UPV/EHU)
Marcelo Caladerón (Polymat and UPV/EHU)

Nanophotonics of 2D materials

January 14-17, 2019
Fudan University, Shanghai, China
http://n2d-2019.dipc.org

Organizing Committee
Hugen Yan (Fudan University, China)
Alexey Nikitin (DIPC, Ikerbasque, Spain)
Tony Low (University of Minnesota, USA)
Luis Martín-Moreno (ICMA, CSIC - Universidad de Zaragoza, Spain)

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

Invited Speakers
Igor Aharonovich (UTS, Australia)
Harry Atwater (Caltech, USA)
Qiaoliang Bao (Monash University , Australia)
Joshua Caldwell (Vanderbilt University, USA)
Qing Dai (NCNST, China)
Michael Fogler (University of California, USA)
Cyriaque Genet (Université de Strasbourg, France)
Irina Grigorieva (University of Manchester, UK)
Alexander Grigorenko (University of Manchester, UK)
Jun He (NCNST, China)
Ping Heng Tan (Institute of Semiconductors, China)
Rainer Hillenbrand (Nanogune, Spain)
Yidong Huang (Tsinghua University, China)
Long Ju (Cornell University, USA)
Frank Koppens (ICFO, Spain)
Maria Maragkou (Nature Materials, UK)
Vinod Menon (City College of NY, USA)
Silvia Milana (Nature Communications, UK)
Yuhei Miyauchi (Kyoto University, Japan)
Timur Shegai (Chalmers, Sweden)
Miriam Serena Vitiello (CNR Nano, Italy)
Chee Wei Wong (University of California, USA)
Jianbin Xu (Chinese University of Hong Kong)
Wang Yao (University of Hong Kong)
Ziliang Ye (University of British Columbia, USA)
Ting Yu (NTU, Singapore)

10th International Meeting on Atomic, Molecular Physics and Chemistry, IMAMPC2019

June 11-14, 2019
CSIC, Madrid
https://imampc2019.wordpress.com/

Organizing Committee
Daniel J. Arismendi-Arrieta (DIPC, Donostia/San Sebastián)
Sergio Díaz-Tendero Victoria (Universidad Autónoma de Madrid)
Cristina Sanz Sanz (Universidad Autónoma de Madrid)

Scientific Committee
Alicja Domaracka (CIMAP, Caen, France)
Edvardas Narevicius (Weizmann institute of Science, Rehovot, Israel)
Graham A. Worth (UCL, London, UK)
Leticia González (University of Vienna, Austria)
Olga Smirnova (MBI, Berlin, Germany)
Paola Bolognesi (ISM, Rome, Italy)
Piotr Zuchowski (UMK, Toruń, Poland)
Rita Prosmiti (IFF, Madrid, Spain)

The meeting is primarily dedicated to young researchers, in the early stage of their scientific careers. In particular, a considerable number of oral presentations will be given by Ph.D. students. The conference is focused mainly on atomic and molecular physics and chemistry (both experimental and theoretical).

Invited Speakers
Alessandra Ciavardini (Italian Synchrotron Elettra Trieste, CERIC-ERIC)
Sandra Gomez Rodriguez (ITC, Universität Wien)
Shirin Faraji (Faculty of Science and Engineering, University of Groningen)
Solene Oberli (Department of Chemistry, UAM)
Daniel Peláez Ruiz (IUT, Université de Lille)
Alvaro Valdés de Luxan (UNAL)
Basile Curchod (Department of Chemistry, Durham University)
David Ayuso (Theory Department, MBI Berlin)
Ignacio Solá (Department of Physical Chemistry, UCM)
Jaroslav Kočišek (Institute of Physical Chemistry, Academy of Sciences of the Czech Republic)
Aleksandar R. Milosavljevic (PLEIADES beamline, Synchrotron SOLEIL, GIF sur YVETTE)
Sadia Bari (DESY)
Loic Journel (LCPMR, Sorbonne Université)
Rui Silva (Department of Theoretical Condensed Matter Physics, UAM)
David Casanova (DIPC)
Rebeca de Nalda (Institute of Physical Chemistry Rocasolano, CSIC)
Joost Bakker (FELIX laboratory, Radboud Universiteit Nijmegen)
Iwona Majewska (Quantum Chemistry laboratory, Uniwersytet Warszawski)
Ewa Erdmann (FTIMS, Gdansk University of Technology)
Sandra Eibenberger (Department of Molecular Physics, FHI Berlin)
Ricardo Pérez de Tudela (Lehrstuhl für Theoretische Chemie, RUB)
Fanny Vazart (IPAG, OSUG)
Julien Eng (School of Natural and Environmental Sciences, NewCastle University)
Inés Corral (Department of Chemistry, UAM)

International Doctoral Training Session - Frontiers of Condensed Matter

September 16-27, 2019
Les Houches, France
https://www.adum.fr/as/ed/page.pl?page=les_houches&site=phys

Organizing Committee
Sebastien Bergeret (DIPC, CFM-CSIC)
Julia Meyer (Université Grenoble Alpes)
Tjerk Oosterkamp (Leiden Institute of Physics/Casimir Research School)
Joerg Schmalian (Karlruher Institut fur Technologie)

This Les Houches international doctoral training session aims at offering Master and PhD students a training program in the area of Condensed Matter Physics. It is organized jointly by the Ecole Doctorale de Physique de Grenoble (France), the Casimir Research School Delft-Leiden (Netherlands), and the Donostia International Physics Center, San Sebastián (Spain). The program consisted of several courses, complemented by more specialized research seminars on timely topics. The school hosted 70 participants, (including lecturers), and was intended for experimentalists and theoreticians.

Topics included:
- Quantum transport.
- Topological phases.
- Quantum information.
- Nanomagnetism.
- Quantum thermodynamics.
- Strongly correlated systems.

Invited Speakers
Y. Nazarov (Delft, Netherlands)
M. Houzet (Grenoble, France)
R. Orus (San Sebastián, Spain)
W. Wernsdorfer (Karlsruhe, Germany)
J. Pekola (Aalto, Finland)
L. Fritz (Utrecht, Netherlands)

3rd Biennial Young Researchers Workshop on Biomaterials and Applications

December 4-5, 2019
Auditorio de Plataforma Tecnológica – Martina Casiano, UPV/EHU Science Park
https://www.biomapp19.org/

Organizing Committee
Mónica Carril (Biofisika, Leioa)
Marek Grzelczak (DIPC, Donostia/San Sebastián)
Fernando López-Gallego (CIC biomaGUNE, Donostia/San Sebastián)
Abraham Martín-Muñoz (Achucarro, Leioa)
Pablo del Pino (CIQUS, Santiago de Compostela)
Pedro Ramos-Cabrer (CIC biomaGUNE, Donostia/San Sebastián)
Javier Reguera (BCMaterials, Leioa)
Luca Salassa (DIPC, Donostia/San Sebastián)

The 3rd Biennial Young Researchers Workshop on Biomaterials and Applications (bioMAPP19) is a scientific meeting focused on biomaterials and their applications in imaging, therapy and sensing. The conference program included Biofunctional Materials, Biosurfaces, Molecular Imaging, Therapy and Diagnosis, and Sensing and Catalysis. BioMAPP19 counted with the participation of 80 young researchers.

Invited Speakers
Lourdes Basade-Desmonts (UPV/EHU)
Pilar López-Larrubia (IIBM, CSIC)
Lucía Gutiérrez (Universidad de Zaragoza)

Higher Education

DIPC School

Nanotechnology meets Quantum Information (NanoQI'19)

July 22-26, 2019
Miramar Palace, Donostia/SanSebastián
http://nanoqi.dipc.org

Organizing Committee
Geza Giedke (DIPC)
Ignacio Cirac (MPI for Quantum Optics, Garching)
Alejandro Gonzalez-Tudela (IFF CSIC Madrid)
Mikhail Lukin (Harvard University)
Atac Imamoglu (ETH Zurich)

Quantum information is at the heart of an ongoing revolution in present-day technology. It is spurred by the increasing control that can be achieved over the quantum state of ever more diverse and complicated systems and the novel paradigms of information processing and sensing enabled by quantum evolution and measurement. The technological importance of this research is evidenced by large public and private investment in the area, including the EU Flagship "Quantum technologies".

A particularly promising direction is to realize this control in nanoscopic systems: nanotechnology structures matter and devices close to or at the atomic limit and approaches now the requisite precision to fully control the quantum state of these structures. This will allow to combine the ultra-small scale factor (and associated advantages in data density and high-speed, low-loss information processing) of nanodevices with the quantum speed-up in computing and sensing.

The NanoQI summer school offered to more than 80 promising young scientists, typically PhD students, from about 22 countries a broad introduction into the state of the art and the major challenges in this rapidly developing research field.

Eight lectures and two research talks focused on three different aspects of the field: On the one hand, on the leading approaches to solid-state-based quantum information processing, covering circuit-QED and superconducting qubits, as well as spin qubits in semiconductor quantum dots and defect centers in diamond and related crystals, highlighting the recent milestones reached in the respective approaches and the challenges faced as experimentalists aim to scale the system up. On the other hand, three lectureres addressed fundamental transversal topics to the field, in particular entanglement theory, the basics of topological quantum computation, and the techniques associated to quantum optics and open quantum systems, which find application in various implementations of QIP. Finally, at the interface of
nanotechnology and quantum informations, were lectures and talks about atomically engineered quantum systems, nanophotonics, and nanoscopic cavity-QED and quantum plasmonics, three areas in which quantum information and nanotechnology are now about to meet, opening new prospects for quantum simulation and ultra-strong light-matter interaction.

In addition to the intense lecture schedule, the participants presented their own work more than 40 posters, which were on display throughout the school, facilitating vibrant and stimulating discussions between all participants.

Invited Speakers
Guido Burkard (Universität Konstanz, Germany)
Yiwen Chu (ETH Zürich, Switzerland)
J. Ignacio Cirac (MPQ Garching, Germany)
Per Delsing (Chalmers University, Sweden)
Barbara Kraus (Universität Innsbruck, Austria)
Javier Aizpurua (CSIC-UPV/EHU, DIPC, Spain)
Klaus Mølmer (Aarhus University, Denmark)
Sander Otte (TU Delft, The Netherlands)
Steven Simon (Oxford University, UK)
Luis Martín-Moreno (ICAM CSIC, Spain)

DIPC School

Topological Matter School 2019

August 19-23, 2019
Miramar Palace, Donostia/SanSebastián
http://tms19.dipc.org

Organizing Committee
Maia G. Vergniory (DIPC, Donostia/San Sebastián, Spain)
Fernando de Juan (DIPC, Ikerbasque, Donostia/San Sebastián, Spain)
Reyes Calvo (Nanogune, Ikerbasque, Donostia/San Sebastián, Spain)
Adolfo G. Grushin (Institut Néel, Grenoble, France)
Erwann Bocquillon (Laboratoire Pierre Aigrain, Paris, France)
Barry Bradlyn (University of Illinois Urbana, Urbana, USA)

The main goal of the Topological Matter School 2019 is to cover material from different approaches to topological matter, showing their relations and differences, in particular in the presence of strong interactions. The school will feature lectures on topological classification, topological insulators, superconductors, and semimetals, the Integer and Fractional Quantum Hall states, anyons and topological order. Over one week, the school will provide extended lectures on these exciting topics by leading experts in both experiment and theory. Students, after the school, will be updated with the last discoveries of the field and a deeper understanding of the fascinating world of topology.

Invited Speakers
Steve Simon (University of Oxford, UK)
Pablo Jarillo-Herrero (MIT, USA)
Moty Heiblum (Weizmann Institute of Science, Israel)
Charlie Kane (Penn, USA)
Frank Pollmann (TU München, Germany)
Michael Zaletel (UC Berkeley,USA)
Vidya Madhavan (UIUC, USA)
Jennifer Cano (Stony Brook , Flatiron Institute, USA)
Alexander Altland (University of Cologne, Germany)
Andrei Bernevig (Princeton University, USA)
Joel Moore (University of California Berkeley, USA)
Leslie Schoop (Princeton University, USA)
Claudia Felser (Max Planck, Dresden)

DIPC School

Machine Learning in Condensed Matter Physics

August 26-28, 2019
DIPC, Donostia/SanSebastián
http://iamc.eu/ML-CM-2019/

Organizing Committee
Maia G. Vergniory (DIPC, Ikerbasque, Donostia/San Sebastián, Spain)
Fernando de Juan (DIPC, Ikerbasque, Donostia/San Sebastián, Spain)
Reyes Calvo (Nanogune, Ikerbasque, Donostia/San Sebastián, Spain)
Adolfo G. Grushin (Institut Néel, Grenoble, France)
Iñigo Aldazabal (CFM-CSIC, Donostia/San Sebastián, Spain)

Complementary to the Topological Matter School celebrated at Miramar Palace, DIPC also organized a satellite course on Machine Learning in Condensed Matter. This after-school course covered the role and application of machine learning in condensed matter physics. In particular, it dealed with machine learning techniques for studying classical and quantum many-body problems encountered in condensed matter, quantum information, and related fields of physics.

Invited Speakers
Lei Wang (Institute of Physics, Chinese Academy of Sciences, China)
Roger Melko (University of Waterloo, Canada)
Eun-Ah Kim (Cornell University, USA)
Zohar Ringel (The Hebrew University of Jerusalem, Israel)

DIPC School

Photo- and ElectroCatalysis at the Atomic Scale (PECAS 2019)

August 27-30, 2019
Miramar Palace, Donostia/SanSebastián
http://pecas2019.dipc.org

Organizing Committee
Sara Barja (CFM-CSIC-UPV/EHU, DIPC)
Celia Rogero (CFM-CSIC-UPV/EHU, DIPC)
Olaf Magnussen (Kiel University)
Doris Grumelli (MPI-FKF, INIFTA – CONICET)

The school on PECAS aims at promoting various opportunities for interdisciplinary discussion of scientists and students of physics, material science, chemistry and electrochemistry in addition to presentation of new results, ideas and methods in the field of photo- and electrochemical properties of novel materials.

PECAS 2019 (second edition) has integrated electrochemistry and surface science research areas and promoted many opportunities for discussion by scientists from both fields and all career stages. The meeting has motivated joyful interdisciplinary interaction from researchers in the surface electrochemistry field, helping to future research collaborations.

Leading experts across the different disciplines have presented their latest experimental and theoretical efforts in the field of photo- and electrochemistry on surfaces, promoting in depth discussions between students and scientific community from both fields.

After the success of the first, and now the second edition of PECAS in 2017 and 2019, respectively, the local organizers have compromised to continue this initiative in Donostia, offering a two yearly meeting held in a truly inspiring environment and promoting the research carry out at the DIPC and CFM centers in this emerging field. The new committee, formed by two local (Sara Barja and Celia Rogero) and two international (Ethan Crumlin and Martin Sterrer) researchers have agreed their compromise for 2021.

Invited Speakers
Marc Koper (Leiden University, Netherlands)
Peter Broekmann (University of Bern, Switzerland)
Ethan Crumlin (Lawrence Berkeley National Laboratory, California)
Elena Savinova (Université de Strasbourg, France)
José Solla Gullón (Universidad de Alicante, Spain)
Nuria López (ICIQ, Spain)
Martin Sterrer (University of Graz, Austria)
Sivan Refaely-Abramsom (Weizmann Institute of Science, Israel)
Maite Alducin (CFM CSIC-UPV/EHU, Donostia/San Sebastán, Spain)
Serhiy Cherevko (HI ERN, Nürnberg, Spain)

DIPC School

Dynapeutics

September 30-October 4, 2019
DIPC and UPV/EHU, Donostia/San Sebastián
http://dynapeutics.dipc.org/

Organizing Committee
Eider San Sebastián (UPV/EHU)
Xabier Lopez (UPV/EHU, DIPC)
David de Sancho (UPV/EHU, DIPC)
Elixabete Rezabal (UPV/EHU, DIPC)
Elena Formoso (UPV/EHU, DIPC)
Rafael Grande-Aztatzi (DIPC)
Jose M. Mercero (UPV/EHU, DIPC)

Dynapeutics international summer school aims to give a theoretical and practical introduction to computational methods for biological molecules, relevant for the understanding of biological processes at the molecular level and especially useful for the design and optimization of molecular drugs. The school is taught at the postgraduate level and is specially addressed to PhD students and postdoctoral researchers with a solid background in biophysics.

Invited Speakers
Emanuele Paci (University of Leeds, UK)
Annick Dejaegere (Université de Strasbourg, France)
Roland H. Stote (Université de Strasbourg, France)
Michael Schaefer (Novartis Pharma AG, Switzerland)
Olivier Michielin (Swiss Institute of Bioinformatics, Switzerland)
Vincent Zoete (Swiss Institute of Bioinformatics, Switzerland)
Antoine Daina (Swiss Institute of Bioinformatics, Switzerland)
Nathalie Reuter (University of Bergen, Norway)
Lennart Nilson (Karolinska Institutet, Stockholm, Sweden)
Leif A. Eriksson (Göteborgs Universitet, Sweden)
Ronen Zangi (UPV/EHU, Spain)
Stefan Boresch (University of Vienna, Austria)
Markus Meuwly (University of Basel, Switzerland)
Maria Joao Ramos (Universidade do Porto, Oporto, Portugal)
Pedro F. Alexandrino (Universidade do Porto, Oporto, Portugal)
Sunhwan Jo (Silcsbio, United States)

DIPC School

Tensor Network Based Approached to Quantum Many-Body Systems (TENSOR19)

November 25-29, 2019
CFM, Donostia/San Sebastián
http://tensor2019.dipc.org/

Organizing Committee
Román Orús (DIPC, Ikerbasque)
Frank Pollmann (Technische Universität München)
Norbert Schuch (MPQ)
Frank Verstraete (Ghent University)

Tensor networks provide a new paradigm for describing quantum many body systems. Since the early years of quantum mechanics, the quantum many body problem has been one of the main driving forces in theoretical physics. In recent years, a lot of progress has been made in unraveling the entanglement structure of correlated systems, which resulted in the study of quantum tensor networks which model the entanglement degrees by local tensors. This had led to the development of new numerical methods for simulating complex quantum systems and of new analytic tools for classifying entangled and topological phases of matter. The aim of the school is to teach young PhD students the basics of tensor-product states as well as the most recent technical developments. It is the 4th school on this topic in the framework of the European Tensor Network initiative, following the success of the previous editions. This is particularly important given the increasing number of groups working on this quickly evolving topic. The lectures will be given by researchers who work actively both on the theory, development and application of tensor-product state based methods.

Invited Speakers
Mari Carmen Bañuls (Max Planck Institute of Quantum Optics)
Román Orús (Donostia International Physics Center)
David Pérez-García (Universidad Complutense de Madrid)
Frank Pollmann (Technische Universität München)
Cecile Repellin (Massachusetts Institute of Technology)
Norbert Schuch (Max Plamck Institute of Quantum Optics)
Sukhwinder Singh (Max Planck Institute for Gravitational Physics)
Frank Verstraete (University of Ghent)

DIPC Course

Dirac and Maxwell equations: Unified view

February, 2019
DIPC, Donostia/San Sebastián

Prof. Iwo Bialynicki-Birula
Center for Theoretical Physics, Polish Academy of Sciences

Even though Dirac and Maxwell equations describe completely different particles: massive charged electrons and massless neutral photons, they have many common features derived from their relativistic character. These common feature not only elucidate the physical properties of photons and electrons but also simplify the generation of solutions of these equations.

The series of three 60 minute lectures were devoted to the description of freely propagating electrons and photons. The course showed how to generate easily various nontrivial solutions and how these solutions are related to the quantum numbers of particles:

- Conceptual differences between relativistic and nonrelativistic quantum mechanics. Relativistic invariance and the related dynamical quantities.
- The relativistic content of the Dirac equation and crucial differences with the Schroedinger-Pauli equation.
- Maxwell equations interpreted as the evolution equation for the photon wave function.

DIPC Course

Density functional theory and time-dependent density functional theory

April, 2019
DIPC, Donostia/San Sebastián

Prof. Luis A. Montero-Cabrera
University of la Habana, Cuba

This course was an introduction to density functional theory and time-dependent density functional theory, with a particular aim at understanding and interpretation of what theory can do and the results of calculations.

The course consisted in 4 lectures of 90 minutes each, held in the DIPC seminar room:

- The density matrix.
- Density functional theory: Concepts. Kohn-Sham approximations. Functionals. Applications to molecular modeling.
- Modeling time dependent electronic processes: Working with Time-Dependent Hamiltonians. Electron excitations as linear response to weak perturbations. Applications of TD-DFT for electron excitations of molecules.

Transdisciplinary Skills Course

On Neurons, Stories and Magic Tricks

July 19, 2019
DIPC, Donostia/San Sebastián

Mario Galarreta
San Francisco, USA

The invited speaker to this special trasndisciplinary lecture, Maria Galarreta is a neuroscientist, a physician, a filmmaker and a mindfulness teacher. After almost 20 years studying the brain, Mario joined Google in 2009, where he worked as a video production manager and led Search Inside Yourself (a mindfulness-based emotional intelligence program). Before Google, Mario was a Senior Research Scientist at Stanford University School of Medicine where he studied the physiology of cortical inhibitory circuits and discovered the existence of gap junctions (electrical synapses) between GABAergic interneurons. Previously, he did a post-doc in Shaul Hestrin's lab at the University of Tennessee, Memphis. Mario was born in Logroño (Spain) and holds an MD (Neurology), a PhD (Ramón y Cajal Hospital, Madrid) and an MFA in Cinema (San Francisco State University). He lives in San Francisco (California) since 2000.

In this lecture, Mario guided the attendants through his trans-disciplinary professional journey, showing us that disciplines that may seem very far from each other, can be more connected than what one can imagine at a first glance.

Transdisciplinary Skills Course

Oral Communication Skills

May-April, 2019
DIPC, Donostia/San Sebastián

Sofi Facal and Manuela Bercioux
Skills for Science and Industry

This course focused on improving the Oral Communication Skills of our young researchers. The course was taught by Sofi Facal and Manuela Bercioux, founders of Skills for Science and Industry. In this course, students developed skills to prepare and deliver high-quality presentations. In particular, the course focused on the following objectives:

- Prepare and structure a short scientific presentation and develop professional presentation material.
- Learn about different audiences and adapt the presentation, its content and message accordingly.
- Use body language and voice successfully during the presentation.
- Get to know and practice different Stress Management Techniques.
- React professionally to questions and feedback after the presentation.
- Formulate professional Questions in a Q&A Session.
- Write and practice a short topic pitch to shortly summarize your work and gain the listener's interest.

The course was structured in 4 sessions of around 4 hours, held in the DIPC seminar room.

Due to the hands-on nature of the course, the lectures were limited to 10-15 students. Anyone in the DIPC community could sign-up for the course, but due to the limited space and according to the formational spirit of the program, PhD students had the highest priority based on a first come first served basis, followed by post-docs and independent researchers.

Theses

Theory of ultrafast electron transfer from localized quantum states at surfaces.
Moritz Müller
05/04/2019
Supervisor: Daniel Sanchez Portal

On-surface synthesis and electronic structure characterization of graphene nanoribbons.
Nestor Merino Diez
12/11/2019
Supervisors: Dimas Garcia de Oteyza and Nacho Pascual

Equilibrium and transport properties of hybrid junctions between superconductors and spin active materials.
Bogusz Bujnowski
27/11/2019
Supervisors: Dario Bercioux and Jerome Cayssol

Master's Degree Program

UPV/EHU Research Master's in Nanoscience

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

The Research Master's in Nanoscience has been offered since 2007 with now 140 students having obtained their Master's degree. Almost 50% of our graduates are international students from four continents (Europe, America, Africa and Asia).

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

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

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