DIPC 2018

Donostia International Physics Center

ON THE COVER OPTICAL TRANSPORT IN DISORDERED MEDIA

Disordered dielectrics can support a photonic band gap in the presence of structural correlations. With the help of numerical simulations, the optical transport in disordered media can be understood and classified according to structural properties. This surprising finding has been published in the context of a collaboration between scientists at the University of Fribourg (Switzerland), the Friedrich-Alexander University of Erlangen-Nürnberg (Germany), and Donostia International Physics Center.

Image Scixel | Enrique Sahagun

Band gap formation and Anderson localization in disordered photonic materials with structural correlations
Luis S. Froufe-Pérez, Michael Engel, Juan José Sáenz, and Frank Scheffold.
Proceedings of the National Academy of Sciences 114, 9570 (2017).

2018

DIPC ACTIVITY REPORT

DIPC: Developing and Sharing Science 4

Board of Trustees 7

Research Activity at a Glance 8

DIPC Supercomputing Center 10

Science Communication 12

Scientific Highlights 21

Publications 55

DIPC Community 88

Researchers 91

Visiting Researchers 107

Personnel 125

Seminars 127

Workshops 137

Higher Education 175

DIPC: Developing and Sharing Science

Donostia International Physics Center (DIPC) is a research center that began its activities in March 2000. The mission of DIPC is to perform and catalyze cutting-edge research in physics and related disciplines, as well as to convey scientific culture to society. Since 2008, the Basque Government's Department of Education has recognized DIPC as a 'Basque Excellence Research Center' (BERC). DIPC is a foundation funded by public institutions (Basque Government, Gipuzkoa Provincial Council, San Sebastian City Council, and the University of the Basque Country) and private companies (currently Kutxa, CAF, Telefónica, and EDP Naturgas Energia) with a common interest in the development of a society and culture based on science.

We have a unique way of operating. DIPC is an agile center that runs under a flexible autonomy of government and management. Researchers are DIPC's center of gravity. DIPC hosts scientists who are knowledgeable, curious, and passionate about their research and provides them with the appropriate grounds to develop their full potential. DIPC is also an international hub between the local community of researchers and a world-wide network of scientists. A constant flow of new ideas is obtained through a program of visiting researchers. This has proven to make a direct impact on the quality of DIPC's research as well as on its international visibility and recognition.

A recent novelty in the life of DIPC has been the diversification of the scientific activity. Until now, research lines at DIPC were mostly focused on several aspects of condensed matter physics, nanoscience, and materials sciences, including the study of advanced materials, attophysics, surfaces and interfaces, photonics, plasmonics, quantum information, polymers, soft matter, biofunctional nanosystems, and computational chemistry, among other topics. The opening of new research lines on experimental particle physics and computational cosmology has enriched the research atmosphere, stimulating creativity in the center as a whole and providing fertile ground for interdisciplinary research. This qualitative growth has been possible thanks to the continuous support of Ikerbasque Basque Foundation for Science.

2018 has been the year in which the DIPC Colloquia started. DIPC Colloquia is a series of colloquium-style talks by outstanding speakers covering all areas of natural sciences. There was an impressive list of contributors during 2018, including Nobel Laureates Francois Englert and Gerard 't Hooft. The informal yet planned gathering of researchers after every talk provides an opportunity for the DIPC scientific community to meet and interact beyond their daily routine.

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

DIPC was conceived and designed based on the idea that an advanced society needs advanced scientific research. Science promotes economic growth, increases productivity and competitiveness, and helps us to live longer and healthier lives. Science also improves our societies in many ways that are not easily measured; it is a successful method to understand our environment. Science tells us that Earth is built from elementary particles of a size unconceivably small. Science tells us that Earth is just a very small planet in a Universe unconceivably big. Science is a necessary tool to confront future challenges in an increasingly complex and interconnected world. Science and the critical thinking intrinsically associated to it are effective antidotes against fundamentalism and intolerance.

As an important part of our mission at DIPC, we assume the responsibility of sharing science. We firmly believe that the spread of scientific culture contributes to the progress and freedom of society. We seek to awaken curiosity, enthusiasm, and passion for knowledge in the general public. For this reason, we develop a broad outreach program that is detailed within this report. Quite often, we create partnerships with other research and cultural institutions to blend different worlds. In 2018 and in collaboration with the Basque Film Archive, we organized a successful cinema cycle that combined movies and science, showing links between both creative activities. In 2019, we will organize a new edition of the "Passion for Knowledge" Science Festival, which has already become an important part of the cultural life of Donostia / San Sebastián.

Last but not least, at DIPC we do not forget that science cannot and must not be disentangled from society. We share the increasing concern about fighting inequality for different social groups. We are therefore committed to design and implement the necessary policies to block out any kind of possible discrimination in the workforce, in particular those related with gender issues. We consider this is simply a matter of justice. We are also committed to promote the progressive use of Open Science practices. We believe that these actions will help us in our mission of developing and sharing more and better science. ■

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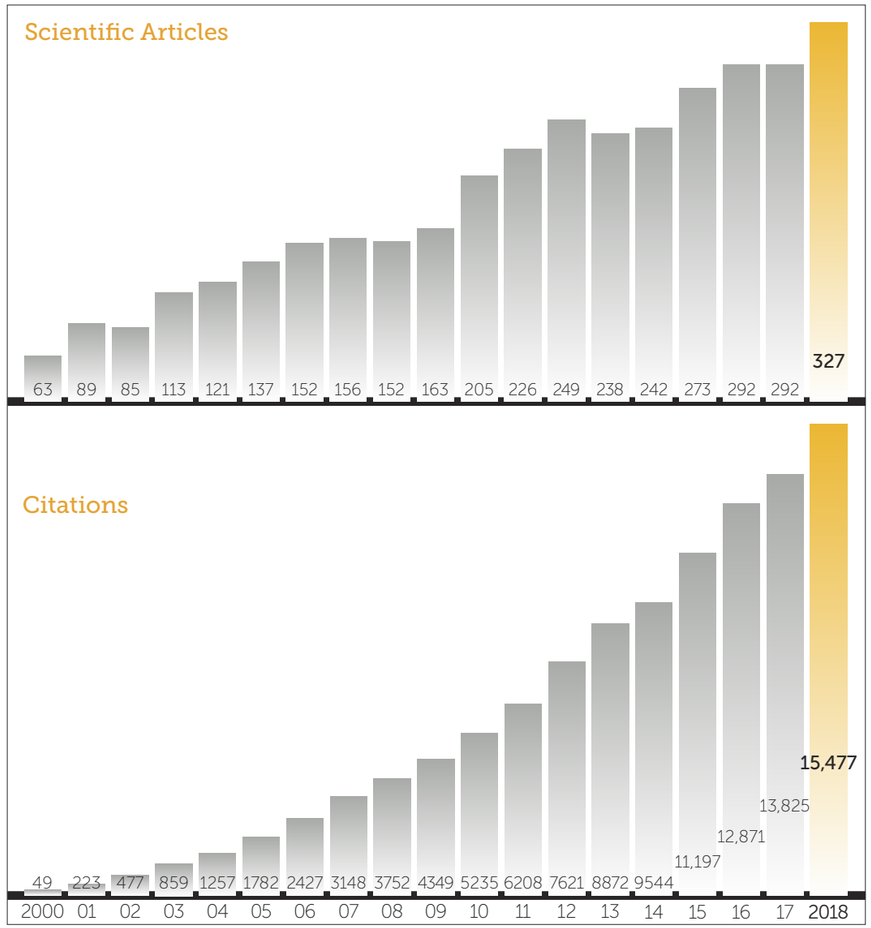
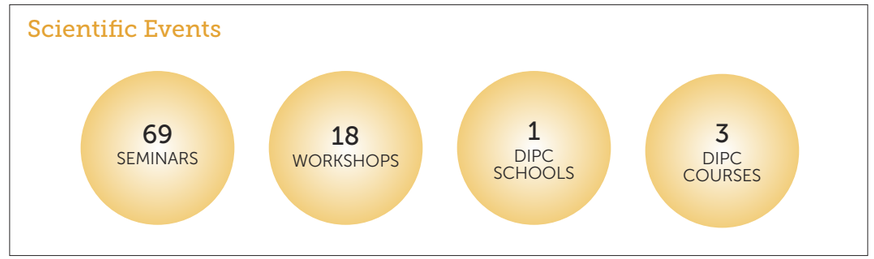
Research Activity at a Glance

DIPC's scientific production and international impact continues to increase. During the last 20 years, the center has published a total of **3,587 ISI publications** and has received more than **109,177 citations**. In 2018, **327 scientific articles** were published, up from 292 in 2016 and 2017.



Source Web of Science Core Collection (all years and indexes) - DIPC's Researcher ID C-3171-2014 (01/04/2019)



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, 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

Computational physics and chemistry are among the strongest research fields in the Basque Country and the Supercomputing Center is one of its key resources. 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.

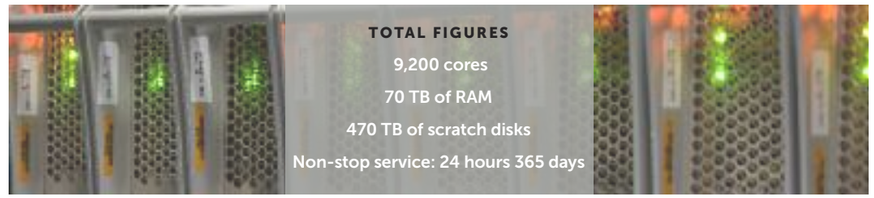
"The variety and power of the computing resources of DIPC, and its constant upgrade, allow the permanent confrontation of a wide range of numerical simulations that put DIPC at the forefront in research.

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 2018, the Center has eight different 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 6,100 cores and 58 TB of RAM, ATLAS is one of the more powerful supercomputers in Spain. In addition, some of our supercomputers have NVIDIA Geforce technology for GPGPU programming or Xeon Phi technology.



More than 180 researchers from DIPC and other research centers such as the UPV/EHU, the CSIC-UPV/EHU Materials Physics Center, CIC nanoGUNE, BioDonostia, several BERCs and Ikerbasque used this computational infrastructure in 2018.

Science Communication

DIPC is fully committed to the dissemination and transfer of scientific knowledge to society because we believe that a more informed society is more prepared to take the decisions that will shape our future. To do so, we establish a fluid and permanent dialogue with society through our extensive outreach program.

Participating students and teachers from around the Basque Country join the speakers and organizers outside Eureka! Zientzia Museoa in Donostia / San Sebastián at the 10th edition of top@DIPC Encounters

top@DIPC Encounters. Zientziarekin solasean!

In 2018 DIPC, in collaboration with Kutxa and Telefónica, organized the 10th annual edition of the top@DIPC Encounters with Nobel laureates, leading researchers, and high school students. The focus of these informal encounters is to foster students' interest in scientific and technological studies. To achieve so, prestigious guest scientists talk about their passion for science and research, and answer questions proposed by participating students about their lives and experiences throughout their careers.

30/10/2018
Eureka! Zientzia Museoa, Donostia / San Sebastián

Klaus Von Klitzing
Nobel Laureate in Physics 1985

Maria Vallet
Chemist and Jaime I Prize in Basic Research 2018

Mairi Sakellariadou
Physicist and cosmologist at King's College London

Presenter:
Idoia Mugica Mendiola
(Materials Physics Center/CFM)
Moderator:
Pedro Miguel Echenique (President of DIPC)

More than **310 students and teachers** from high schools in the Basque Country participated in this year's Encounter. **Telefónica**, a long-time patron of DIPC, collaborated by giving two awards to students asking the most innovative, creative, and surprising questions.

Bergara: EPS Historic Site

In 2017, DIPC made a presentation to the European Physical Society (EPS) defining the scientific and historical relevance of the Laboratorium and the Seminary of Bergara in the discovery of wolfram (tungsten). The Elhuyar brothers isolated wolfram for the first time in 1780. The City Council of Bergara and DIPC worked together to obtain the distinction of "EPS Historic Site" which commemorates places in Europe important for the development and the history of physics.

On October 20, 2018, **Iñigo Urkullu**, Lehendakari (President) of the Government of the Basque Country and **Markel Olano**, Deputy General of Gipuzkoa, **Elena Lete**, Mayoress of Bergara, along with **Rudiger Voss**, President of the EPS, **Pedro Miguel Echenique**, President of DIPC, participated in the act. The Minister of Education, **Cristina Uriarte** and the Rector of the University of the Basque Country (UPV/EHU) **Nekane Balluerka** attended the historic event.

More than 80 international scientists who participated in the HOPDSS2018 workshop on the history of physics organized by DIPC and the EPS at the Miramar Palace in Donostia/ San Sebastián, were invited to Bergara as well. In total, more than **250 people participated in the event**.

OUT THERE
Cinema and Science

In 2018, DIPC in collaboration with the Basque Film Library and Azkuna Zentroa of Bilbao, organized a Cinema and Science series entitled 'Out There' with the theme of space exploration and search for extraterrestrial life as a guiding thread. In each of the sessions, a guest scientist contextualized the film and analyzed the greater or lesser scientific rigor of it in relation, among other things, to the historical moment in which it was filmed. Apart from the film, a lecture was given about the universe. Sessions for scholars were also organized.

Films projected in
Donostia / San Sebastián and Bilbao

Interstellar (Christopher Nola, 2014)
*The day the Earth stood still (*Robert Wise, 1951)
*Forbidden planet (*Fred McLeod Wilcox, 1951)
Arrival (Denis Villeneuve, 2016)
E.T. The Extra-terrestrial (Steven Spielberg, 1982)
Invasion of the body snatchers (Don Siegel, 1956)
Gravity (Alfonso Cuarón, 2013)
Alien (Ridley Scott, 1979)
The Martian (Ridley Scott, 2015)
The War of the Worlds (Byron Haskin, 1953)

Invited scientists

Pedro Miguel Echenique
Professor at UPV/EHU / President of DIPC

Marian Iriarte
Professor at UPV/EHU / Dean of the Faculty of Chemistry

Amaia Esquisabel
Researcher in pharmaceutical technology / Research director of the Basque Government

Juan Ignacio Cirac
Physicist / Director of the Max Planck Institute of Quantum Optics

Itziar Laka
Linguist / Professor at UPV/EHU

Javier Aizpurua
Physicist / CSIC research professor and director of CFM (CSIC-UPV/EHU)

Rafael Yuste
Neurobiologist / Professor of Biological Sciences and Neuroscience at Columbia University and co-director of the Kavli Institute for Brain Science

Ruth Lazkoz
Cosmologist / Lecturer at UPV/EHU

Igor Campillo
Physicist / Director of Euskampus Fundazioa

Rafael Rebolo
Astrophysicist / CSIC research professor and director of the Canary Islands Institute of Astrophysics

Fernando Cossio
Chemist / Professor at UPV/EHU and director of Ikerbasque

Naia Pereda
Physicist / Radiotherapy Unit from Basurto University Hospital

Agustín Sánchez-Lavega
Astrophysicist / Professor at UPV/EHU

Txomin Romero
Computer engineer / Director of DIPC Supercomputing Center

Public Lecture
22/02/2018
La gravedad y el universo:
desde los sistemas planetarios y los agujeros negros al Big Bang

Rafael Rebolo, Astrophysicist and director of the Institute of Astrophysics of the Canary Islands, gave a public talk about the Universe for all audiences in Donostia / San Sebastián, followed by the screening of *Gravity*.

Special projections for schools
In addition, special projections of *The Martian* were organized within the cycle, aimed at schools in the Basque Country in collaboration with the Planetary Sciences group of the University of the Basque Country (UPV/EHU). The events took place the 17th and 19th of January in Tabakalera, Donostia / San Sebastián, and the 5th of February at Azkuna Center, Bilbao. After the screening of the film, astrophysicists Naiara Barrado-Izagirre and Santiago Pérez-Hoyos gave their insight into martian exploration by introducing the planetary research projects in which they are immersed.

The success of attendance at the 18 scheduled sessions between Donostia / San Sebastián and Bilbao, in addition to the specific sessions for high school students, totals close to 3000 spectators.

On Zientzia

DIPC and Elhuyar Foundation organized the 8th edition of the ON ZIENTZIA video contest which promotes the production and diffusion of short and original videos encouraging positive and progress values of science and technology. The award ceremony took place on the 12th of June at Tabakalera International Centre for Contemporary Culture (Donostia / San Sebastián). The event was later broadcast on Teknopolis, a local TV program. 80 videos were entered into the contest.

BEST DISSEMINATION VIDEO
Vacuum
Patxi Razkin Senar (Engineer at CAF)

BEST VIDEO IN BASQUE
Vulkano, gizateriaren margolari
Jon Puignau (High school teacher)

YOUNG PRIZE
¿Cómo hacer una bomba atómica?
Adrián Gálvez Pantoja (16 years old)

SPECIAL MENTIONS
¿Qué es eso de la elasticidad?
María Miguélez
Virus como armas contra bacterias patógenas
Diana Gutiérrez Fernández and Lucía Cornejo Villanueva

For more information visit:
www.onzientzia.tv

Bertsozientzia

Bertsozientzia is an initiative that seeks to merge two seemingly distant disciplines such as science and bertsolaritza. Organized by the Chair of Scientific Culture of the UPV/EHU, in 2018, its fourth edition was programmed and held for the first time in Gipuzkoa thanks to DIPC.

The Zarautz On Association, Laboratorium Museum of Bergara, Lemniskata Goierriko Zientzia Sare Herrikoia net, together with the City Councils of Bergara, organized the event which took place in Zarautz, Bergara and Ordizia on May 15, 17 and 25, respectively.

Entitled "Jakinduriek Mundue Erreko Dau" (Knowledge will burn the world), the evenings brought together three scientists and two bertsolaris on the same stage. The program was made up of 10 minute scientific talks in Basque. After the exposition, the bertsolaris faced the challenge of improvising a bertso that picked up the hypothesis put forward by the scientist. The response from the public was very positive with 225 participants in Zarautz, 175 in Bergara 175 and 150 in Ordizia.

15/05/18 | ZARAUTZ
Bertsolaris:
Maialen Lujanbio
Aitor Sarriegi
Scientists or researchers:
Ainara Sangroniz
Félix Zubia
Josu López Gazpio

17/05/18 | BERGARA
Bertsolaris:
Andoni Egaña
Miren Amuriza
Scientists or researchers:
Ainara Sangroniz
Jon Mattin Matxain
Gorka Azkune

25/05/18 | ORDIZIA
Bertsolaris:
Unai Iturriaga
Alaia Martín
Scientists or researchers:
Gorka Azkune
Olatz Pérez de Viñaspre
Aitor Gastañares

New Ways of Science Lecture

These talks organized jointly by Ernest Lluch Cultural Center from Donostia Kultura and DIPC in an attempt to bring our work closer to society. Scientists from DIPC introduce the fundamentals of Materials Science and historical milestones in a clear and attractive way to the general public. In 2018, we organized the following lecture:

17/04/2018
Introducción a la visión artificial y sus retos actuales
Ignacio Arganda Carreras
Ikerbasque Research Fellow, Department of Computer Science and Artificial Intelligence, Faculty of Informatics (UPV/EHU) and DIPC Associate

nanoKOMIK

nanoKOMIK is a project promoted by DIPC and CIC nanoGUNE to raise awareness of the potential of the advances made in nanoscience. The project was launched in 2016 structured in two phases: a first phase in which a challenge aimed at young people is proposed to create a nanofiction comic, and a second, in which, with the help of cartoonists, the best ideas emerged in the challenge are recreated.

nanoKOMIK is carried out in four languages — Basque, Spanish, French and English— and the project established new cross-border collaborations in the field of scientific dissemination between France and Spain.

Itinerant exhibition

The itinerant exhibition of the collective comic *nanoKOMIK* has made the following journey during 2018:

23/10/2017–09/02/2018
Komikigunea, Koldo Mitxelena Zentroa, Donostia / San Sebastián

20–26/09/2018
Centro de Iniciativas Culturales de la Universidad de Sevilla

22–26/10/2018
WEEK INN Semana de la Innovación, Donostia / San Sebastián

30/10–04/11/2018
ZTB Zientzia, Teknologia eta Berrikuntza Astea, Sala Aroztegi, Bergara

8–10/11/2018
Science Week, UPV / EHU, Tabakalera, Donostia / San Sebastián

In addition, the comics created from the two challenges (2016, 2017) have continued to be published in the *Jot Down Kids* magazine, which is distributed with the national newspaper El País.

By the end of 2018, we have started translating the comic books into Korean through the collaboration that DIPC maintains with the Center for Quantum Nanoscience in Seoul.

Science Week
08–10/11/2018

Master's and 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 Material's World' at the Science Week organized by the University of the Basque Country (UPV/EHU). In addition to the stand, the itinerant exhibition of nanoKOMIK was exhibited in an adjacent area prepared for this purpose.

In Praise of Science and Culture

Pedro Miguel Echenique, founder and president of DIPC, continues to play an active role in raising awareness of the necessity and importance of basic research for the development of society and culture. During 2018 Professor Echenique delivered 15 lectures locally and internationally in a variety of events.

NAUKAS DONOSTIA, de lo pequeño a lo grande

19/05/2018
Victoria Eugenia Theater
Donostia / San Sebastián

Naukas Donostia, from the small to the big is a series of lectures given by prestigious scientists and acclaimed science disseminators. A journey was made through the scales of the Universe, starting with nano-technology, to the largest objects that we know.

This walk through the scales and sizes of the Universe was divided into two sessions; morning and afternoon, with a total of 12 talks of 25 minutes each. Approximately 350 people attended both the morning and the afternoon sessions.

In addition, the event was streamed live and followed by 837 people.

To watch the videos visit:
www.eitb.eus/es/divulgacion/

TALKS

Pedro Miguel Echenique De lo pequeño a lo grande
De lo simple a lo complejo

Juanjo Gómez Cádenas La sublime utilidad de los inútiles neutrinos

Sara Barja Papiroflexia a la 10-9

Javier Aizpurua Ver o no ver, esa es la cuestión

Ignacio López Goñi Viven en comunas, son cotillas y muy promiscuas

Almudena M. Castro Sonidos pequeños, grandes y aterradores

Juan Ignacio Pérez Grandes y pequeños

Aran Garcia Lekue Surf: ciencia y serendipia

Ricardo Hueso Diversidad planetaria

Beatriz Sevilla ¿Qué es esa cosa borrosa en el cielo?

Miguel Santander ¡Dios mío, está lleno de Galaxias!

Natalia Ruiz / Manuel González De lo pequeño a lo grande: the overview

Mestizajes
Crossing the boundaries among Art, Science and Humanities

Mestizajes is a project coordinated by **Gustavo Ariel Schwartz**, researcher at the Materials Physics Center (CFM) and associated to DIPC, aimed at all audiences and designed with an innovative and original perspective to promote dialogues between science, literature and humanities. The project is promoted and organized by DIPC within the framework of Euskampus, Campus of International Excellence. *Mestizajes* is a space which promotes intellectual diversity and hybridization between different forms of knowledge.

TALKS

The talks were held at DIPC with the aim of introducing into the scientific community the debate about creativity.

11/10/2018
Tomás Saraceno:
The art and science of cosmopolitics
Joanna Page
University of Cambridge, UK

31/10/2018
Poincaré en la orilla:
observaciones sobre la invención científica
Francisco González Fernández
Oviedo University, Spain

Science Dissemination Contest

Organized annually since 2015 in collaboration with the well-known Spanish cultural magazine *Jot Down*, the contest recognizes the best science dissemination articles. Within the framework of the Science Jot Down event, each year the best scientific dissemination articles submitted to the contest are recognized. The award ceremony took place on the 22th of September in Seville with the following winners:

FIRST PRIZE
El detective que bebía whisky con hielo
Oskar González García

SECOND PRIZE
El regalo de Hitler
José Ramón Alonso

High School Visits

In 2018, DIPC together with the Materials Physics Center (CFM) continued the program of visits for groups of high school students launched in 2014. Both centers open their doors so these young students can meet researchers and view their work up close.

Between 2014 and 2018, 1592 students from 55 schools visited our center. During the 2018/19 academic year, 474 students from 14 schools will visit DIPC during the months of October and June.

Scientific Highlights

Similar temperature scale for valence changes in Kondo lattices with different Kondo temperatures 22

Directional control of light–matter interactions at the nanoscale 24

Catalytic oxidation of carbon monoxide on a curved Pd crystal: spatial variation of active and poisoning phases in stationary conditions 26

Spin control using chemical design 28

Polariton anomalous hall effect in transition-metal dichalcogenides 30

Nanoalloying MgO-deposited Pt clusters with Si to control the selectivity of alkane dehydrogenation 32

Observation of topologically protected states at crystalline phase boundaries in single-layer WSe_2 34

Chirality-induced electron spin polarization and enantiospecific response in solid-state cross-polarization nuclear magnetic resonance 36

Bioorthogonal catalytic activation of anticancer metal complexes 38

Coupling of molecular emitters and plasmonic cavities beyond the point-dipole approximation spectroscopy 40

Living nanospear for near-field optical probing 42

Survival of spin state in magnetic porphyrins contacted by graphene nanoribbons 44

The attosecond streaking with rotating THz field 46

Degradability of fermionic gaussian channels 48

Bottom-up synthesis of multifunctional nanoporous graphene 50

Atomic-scale lightning rod effect in plasmonic picocavities: a classical view to a quantum effect 52

DIPC HIGHLIGHT 2018

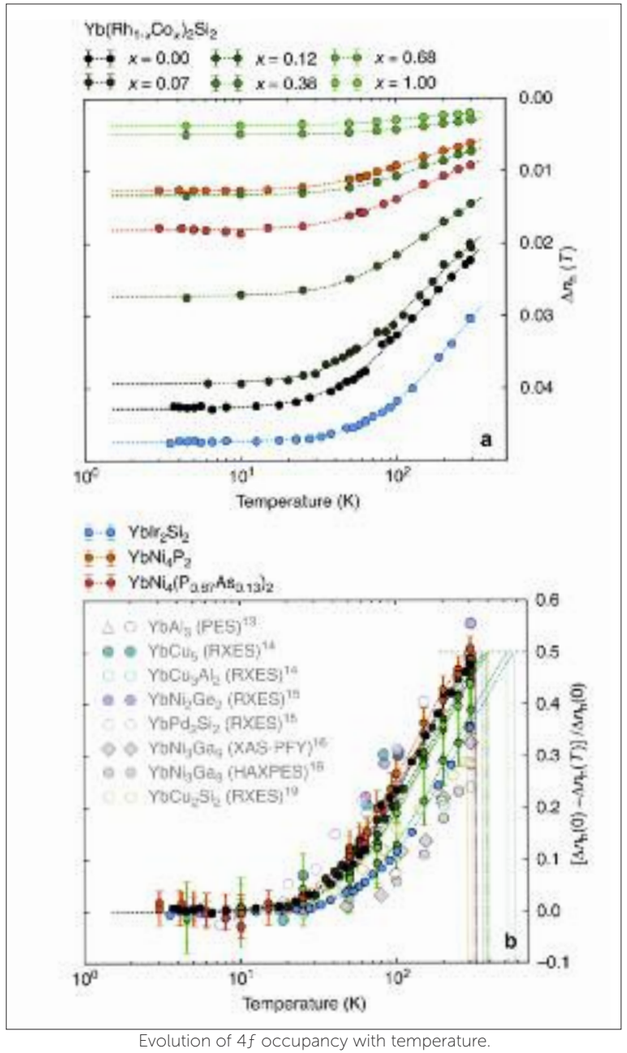
Similar temperature scale for valence changes in Kondo lattices with different Kondo temperatures

Kummer K, Geibel C, Krellner C, Zwicknagl G, Laubschat C, Brookes NB, and Vyalikh DV.
Nature Communications 9, 2011 (2018)

The interaction of localized electrons in a bath of itinerant ones is a source of exotic physical phenomena ranging from magnetic order to superconductivity to Kondo and heavy-fermion states and even to a break-down of the Fermi-liquid picture. These properties show up in more and more materials and could play an important role in future applications. Therefore a lot of efforts are made in order to gain a profound understanding of the interplay between localized and itinerant electrons.

For many years now, our team has concentrated on disentangling and understanding the temperature dependent electronic properties in rare-earth based strongly correlated electron systems. Here, we report a surprising and strongly unexpected experimental result related to the Kondo effect. We explicitly demonstrate that in agreement with the predictions of the Kondo model the zero temperature occupation of the 4f level scales with the Kondo temperature of the system. However, in stark contrast to expectations based on the Kondo model the evolution of the occupation of the 4f level with temperature is independent of the Kondo temperature and seems to occur on the same temperature scale for all Yb Kondo lattices. Our results demonstrate that the temperature dependence follows a universal curve that perfectly fits our data and data reported by other research groups. We believe that this clear failure of the current approaches to Kondo physics has only been seen now because this is the first X-ray spectroscopy study that included a larger number of Kondo lattice systems with a wide range of Kondo temperatures from as low as 0.25 K to as high as 500 K. We started out 6 years ago and have performed a series of synchrotron experiments to obtain and confirm the unique and unexpected results presented here.

Our experimental observation shows that the general understanding of the Kondo phenomenon, is still far away from being complete and clear. Analyzing possible origins of this unexpected universal T scaling, we identify two possible candidates, thermally excited crystal-electric-field (CEF) levels and lattice vibrations. The effect of both properties on n(T) has hardly been discussed yet and is far from being clear at the moment. Our results urge for more experimental studies on how excited CEF levels and lattice vibrations affect the T dependence of the valence in Yb Kondo lattices. They also show very clearly that further advances in theoretical approaches to the Kondo model are needed. The simple approximations used so far have been successful in describing even fine details of some physical properties of Kondo lattices but clearly fail to capture others as demonstrated by our experiment.



Evolution of 4f occupancy with temperature.

The competition between interactions promoting magnetic order and those supressing magnetism causes unusual electronic behaviour in Kondo lattice materials. Here, the authors show the energy scale for valence fluctuations is not controlled by the Kondo scale, contrary to expectations from single-site models

DIPC HIGHLIGHT 2018

Directional control of light–matter interactions at the nanoscale

Ma WL, Alonso-Gonzalez P, Li SJ, Nikitin AY, Yuan J, Martin-Sanchez J, Taboada-Gutierrez J, Amenabar I, Li PN, Velez S, Tollan C, Dai ZG, Zhang YP, Sriram S, Kalantar-Zadeh K, Lee ST, Hillenbrand R, and Bao QL.
Nature 562, 557 (2018)

DIPC participates in the discovery of squeezed infrared light in the nanoscale that propagates only in specific directions along thin slabs of molybdenum trioxide – a natural anisotropic 2D material. Besides its unique directional character, this squeezed light "lives" for an exceptionally long time, and thus could find applications in signal processing, sensing or heat management at the nanoscale.

Future information and communication technologies will rely on the manipulation of not only electrons but also of light at the nanometer-scale. Squeezing light to such a small size has been a major goal in nanophotonics for many years. An international team of researchers, including Ikerbasque Research Associate, Alexey Nikitin (DIPC), has published in Nature a breakthrough in nanophotonics that could deliver exactly that: particularly strong light confinement. The scientists claim that such confinement can be achieved with phonon polaritons – quasiparticles resulting from the strong coupling of photons with a dipole-carrying atomic lattice vibrations –, existing at infrared frequencies in in thin slabs of α-phase molybdenum trioxide (α–MoO3), a natural van der Waals polar semiconductor. Apart of the remarkable electromagnetic fields confinement, these phonon polaritons propagates only in specific directions, thus being essentially anisotropic. The team has realized that under the extreme anisotropy phonon polaritons in α–MoO_3 can become "hyperbolic", making the energy and wave-fronts to propagate in different directions along the surface of the crystal slab, which can lead to interesting exotic effects in optics, such as e.g. negative refraction or superlensing. Besides their unique directional character, the polaritons live for the record long time at the room temperature, thus opening exciting possibilities for the strong electromagnetic coupling between polaritons and molecules.

The reported results not only add a new member to the growing list of polaritons in van der Waals materials. In combination with external stimuli, such as strain, electric gating or photo-injection of carriers, it is conceivable that the active tuning of the properties of the anisotropic phonon polariton is within reach. These findings may thus establish a route to the directional control of light and light–matter interactions at the nanoscale.

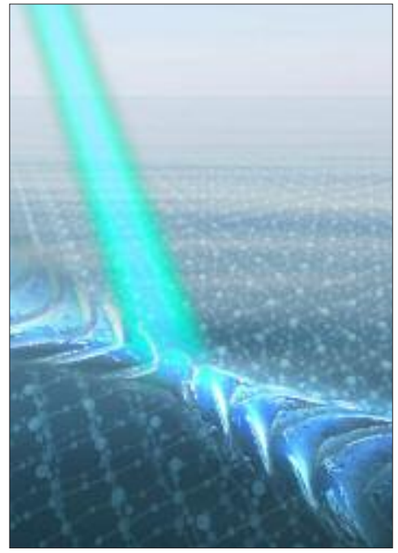


Figure 1. An artistic representation of phonon polaritons in α-MoO_3, excited by a laser beam.

Our results show that polaritons on α–MoO_3 live up to 20 picoseconds, which is 40 times larger than the best-possible polariton lifetime in high-quality graphene at room temperature

Our findings promise α–MoO_3 to become a unique platform for infrared nanophotonics

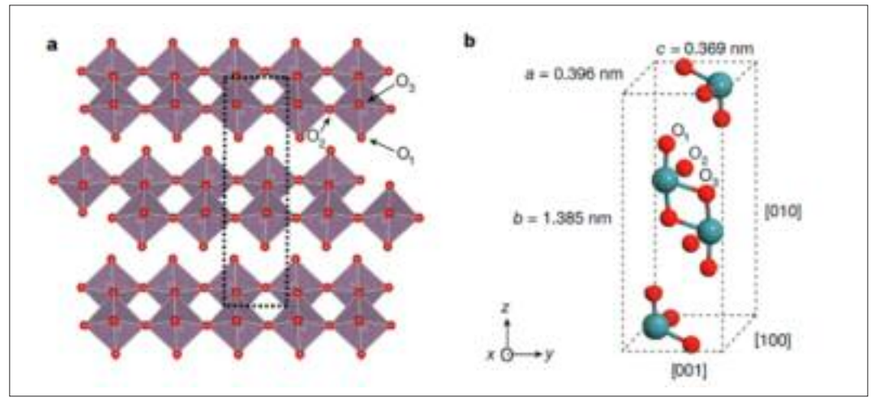


Figure 2. a) The orthorhombic lattice structure of layered α-MoO_3 (red spheres, oxygen atoms). b) The unit cell of α-MoO_3

DIPC HIGHLIGHT 2018

Catalytic oxidation of carbon monoxide on a curved Pd crystal: spatial variation of active and poisoning phases in stationary conditions

Schiller F, Ilyn M, Perez-Dieste V, Escudero C, Huck-Iriart C, del Arbol NR, Hagman B, Merte LR, Bertram F, Shipilin, M, Blomberg S, Gustafson J, Lundgren E, and Ortega JE.
Journal of the American Chemical Society 140, 16245 (2018)

The CO oxidation reaction was stopped at fixed temperature and pressure on a curved palladium crystal surface, and then active surface and gas species were probed with Near Ambient Pressure Photoemission. Results straightforwardly demonstrate the substrate-dependent character of the CO oxidation ignition and, more important, the coexistence of active and poisoning surface chemical phases within a sizeable temperature range.

Carbon monoxide (CO) oxidation ($2CO + O_2 \rightarrow CO_2$) on platinum group metal surfaces is a model heterogeneous gas/surface catalytic reaction with enormous technological impact in car industry. Despite its importance, there is no consensus on how this reaction actually proceeds at the "ignition" point, that is, what is the nature of chemical species and their interplay with the crystal structure at the surface of the catalyst when it becomes active. With the advent of analytical techniques that operate under realistic reaction conditions, such as Near Ambient Pressure X-ray Photoemission (NAP-XPS) this important catalytic process has been lately re-examined on a variety of crystal surfaces of transition metals, such as palladium, aiming at understanding the catalytic performance of the different crystal planes that shape technologically relevant nanoparticles.

The cylindrical Pd crystal schematically depicted in Figure 1 defines a smooth variation of the crystal orientation at its surface, allowing us to carry out a straightforward comparative study of the catalytic activity of different Pd crystal planes in NAP-XPS. The curved direction spans the complete set of vicinal orientations for the two type of close-packed atomic steps (called A and B) around the (111) symmetry direction. Since the radius of curvature of the sample is three orders of magnitude larger than the X-ray light spot in synchrotron ALBA (Barcelona), separate crystallographic planes can be sequentially probed by scanning the X-ray photon beam in XPS.

In this work published in *JACS 2018, 140, 16245* we have driven the Pd curved sample of Figure 1 to stable reaction conditions at fixed temperatures around the ignition point, and have used NAP-XPS to identify the sequence and evolution of surface chemical species across the different crystal planes of the surface.

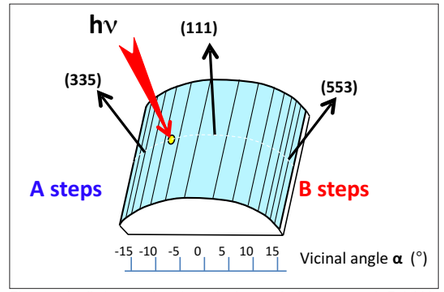


Figure 1. Schematic description of the curved Pd(111) sample used to simultaneously probe, via Near Ambient Pressure Photoemission, the catalytic activity of different Pd crystal planes in the CO oxidation reaction.

Using a curved crystal sample, chemical species during the ignition of the CO oxidation reaction are imaged at different Pd crystal planes

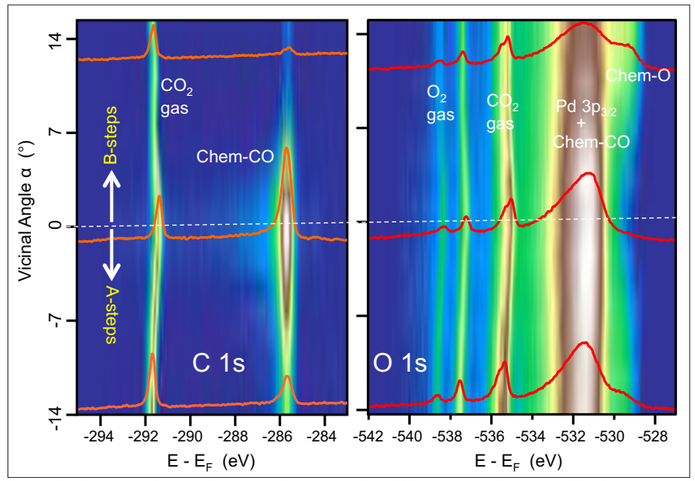


Figure 2. Map of surface and gas species across the different crystal planes (vicinal angle α) of the curved Pd(111) sample, measured under stationary temperature (485 K) and pressure (0.5:0.5 mbar of $CO:O_2$) conditions. The variable balance of chemisorbed CO and oxygen-related species indicate that both may coexist and that the ignition process depends on the local crystal plane.

The result is a consistent description of the surface chemistry during the catalytic oxidation of CO on Pd(111) and its vicinal planes. As a way of example, Figure 2 shows the map of chemical species at 485 K as a function of the local crystal plane (vicinal angle α). We observe a strong spatial variation in the balance of poisoning (CO-related) and active species (oxygen-related), which demonstrates, first, that both poisoning and active species can coexist and, second, that the reaction is activated in the local plane and at different temperatures, with a clear A–B asymmetry. Two parameters appear to be responsible for this latter: the α-dependent variation of the CO chemisorption energy and the structural transformation of the surface, likely oxygen-induced faceting, beyond critical vicinal angles.

DIPC HIGHLIGHT 2018

Spin control using chemical design

Karan S, Garcia C, Karolak M, Jacob D, Lorente N, and Berndt R.
Nano Letters 18, 88 (2018)

The affinity of ligand groups can change the magnetic moment of a molecule by capturing charge from a metallic environment

Iron porphyrin is a magnetic molecule with a magnetic moment of two Bohr magnetons (two unpaired electrons). The magnetism is due to the Fe atom in the ligand field controlled by 4 N atoms. However, the enviroment of these atoms matter. Here, it is shown that by changing the far ends of the molecule, the magnetic core changes its nature, due to the unified structure of the molecule.

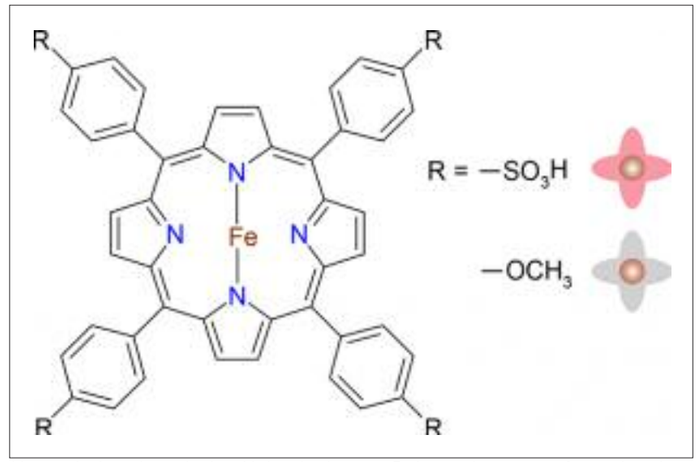
The scanning tunneling microscope (STM) consists of a metallic tip that is biased with respect to a metal substrate. On the metal substrate different types of Fe-porphyrin molecules are adsorbed. The difference between the molecules is a different ending R group. The STM tip is specially etched to have a sharp apex that has to be atomically ended to be able to reach submolecular resolution, as the one obtained in the experiments.

The STM can fix the tip at a certain distance from the molecule, and change the bias. The tip-to-molecule distances are about 0.5 nm and rarely go above 1.0 nm. These range of distances are usually far enough to avoid direct chemical interactions between tip and molecule, but short enough to be able to measure the tiny electronic currents involved. In these conditions, one can measure the differential conductance. This is the derivative of the current with respect to bias at different biases. When the bias is large enough to produce some excitation, the tunneling electron yields energy to the excite the molecule. The tunneling electron has then two possibilities, either excite the molecule or tunnel without excitations. The current increases a this threshold, and if you take the derivative you see a step in the conductance.

A magnetic molecule like these Fe porphyrins contains magnetic excitations that correspond to changing the orientation of the Fe magnetic moment, unless there is only one unpaired electron. In this last case we have a spin ½ system. A quantum-mechanics property of a spin ½ is that it is totally isotropic: the energy is the same wherever the magnetic moment is pointing at.

The differential conductance of the two different R groups is very different. In one case, there are clear steps of a magnetic excitation. This is compatible with the two unpaired electrons of the classical Fe porphyrin. However, when the group is donating electrons, the differential conductance does not show a step, indicating that this is rather a spin ½ system. The R group is capable of changing the magnetic moment of the molecule.

These results can be understood in the following way: when the R group is OCH_3, the group does not pull charge from the substrate, and the molecule maintains its gas-phase magnetic moment; however, when the group is SO_3H, the full electron affinity of the molecule increases, and there is net electron transfer from the substrate into the molecule that leads to a reduction of unpaired electrons and of the molecular magnetic moment.



Meso-substituted porphyrins. Molecules host an Fe ion at the center of tetraphenylporphyrin with four *meso*-subgroups occupying para positions of the phenyl rings. H atoms are not shown. Phenyl rings are substituted with sulfonyl hydroxide ($–SO_3H$) or methoxy ($–OCH_3$) groups. The magnetic properties of the molecule are localized at the Fe core, but the nature of the distant R group radically changes the value of the molecular magnetic moment despite the fact that the R groups are not magnetic.

DIPC HIGHLIGHT 2018

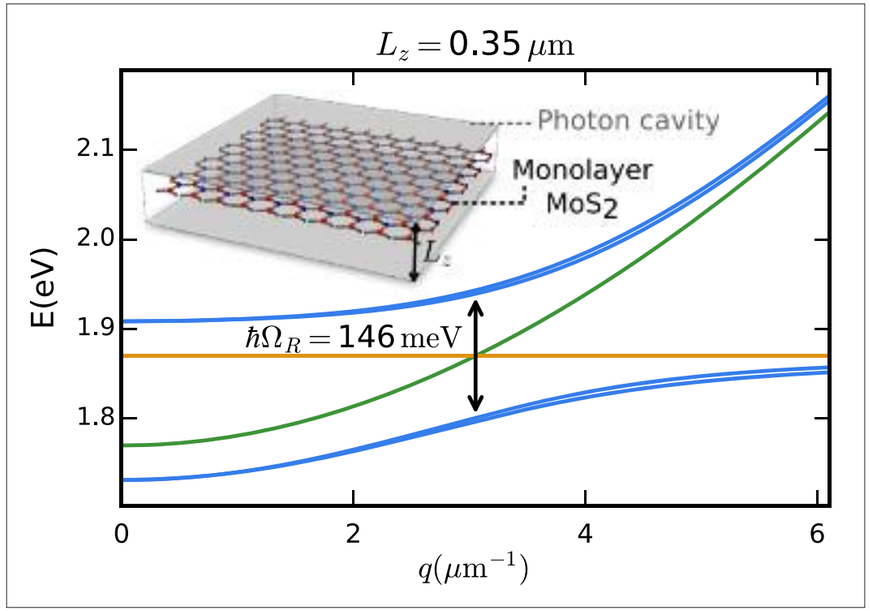
Polariton anomalous hall effect in transition-metal dichalcogenides

Gutierrez-Rubio A, Chirolli L, Martin-Moreno L, Garcia-Vidal FJ, and Guinea F.
Physical Review Letters 121, 137402 (2018)

Two-dimensional materials, such as transition-metal dichalcogenides embedded in optical cavities, stand out as an excellent platform where the combined effect of topology and strong light-matter coupling can be studied and utilized. In this theoretical work, a team of researchers from different institutions, including DIPC, reports on the possibility of inducing a polariton anomalous Hall effect in this type of structures.

When the interaction between light (vacuum field) and matter (an exciton formed from a bound electron-hole pair in a crystal) in very strong, hybrid light-matter quasiparticles named as polaritons emerge. A striking property of these polaritons is that they inherit the huge velocity of its light component and the interactive character of its matter part, the best of the two worlds. On the other hand, topological insulators are electronic materials that have a bulk band gap like an ordinary insulator but have conducting states on their edge or surface. The important point of these new materials is that electronic transport by the conducting states is protected due to spin-orbit interactions that break time-reversal symmetry. In standard materials, the usual way of breaking time-reversal symmetry is by utilizing an external magnetic field. Amongst many others, one of the practical implications of this topologically-protected electron transport is the feasible realization of the quantum Hall effect but without the need of an external magnetic field, what is called an anomalous quantum Hall effect.

In this publication, a team of researchers has studied strongly-coupled excitons and photons (polaritons) in a monolayer of MoS_2, a transition-metal dichalcogenide, embedded in a Fabry-Perot cavity. In a similar way as the spin-orbit interaction does in electronic topological insulators, it is found that the cavity itself promotes/induces a selection-rule breaking in the propagating characteristics of the polaritons. In this way, light-matter coupling due to the cavity is able to open a gap in the polaritonic dispersion relation. This results in a splitting of the topological charge of the polariton, which is not present in either of its constituents (exciton and photon). As a way of example, the researchers propose to visualize this effect by realizing a polariton anomalous Hall effect, in which two polaritons could be deviated in opposite directions depending on their topological charge.



Excitons in a MoS_2 monolayer embedded in a planar optical cavity are studied in this work (inset). The graph represents the dispersion relation of a bare exciton and a photon in a cavity and the two resulting polaritonic branches in the strong-coupling regime.

The detailed microscopic analysis of the exciton-photon coupling in a MoS_2 monolayer embedded in an optical cavity reveals highly tunable features of the spectrum that result in polariton splitting and a breaking of light-matter selection rules

DIPC HIGHLIGHT 2018

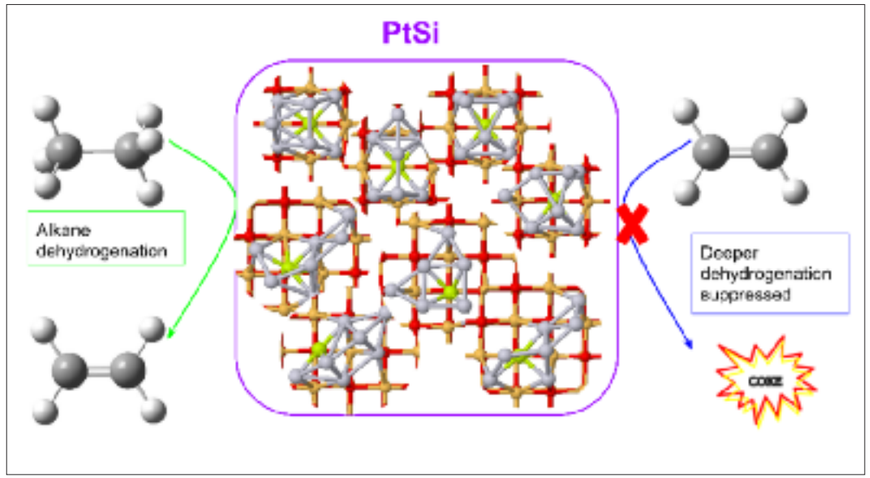
Nanoalloying MgO-deposited Pt clusters with Si to control the selectivity of alkane dehydrogenation

Jimenez-Izal E, Zhai HC, Liu JY, and Alexandrova AN.
ACS Catalysis 8, 8346 (2018)

Although platinum is the most active pure metal for the dehydrogenation of light alkanes, to produce light olefins, it deactivates with time-on-stream due to severe coke deposition and sintering or thermal deactivation of small nanoparticles. In the present work we show that doping platinum with silicon can improve the sintering and coking resistance, and therefore, create a more robust catalyst with longer lifetime.

Light olefins are among the most important organic molecules, with the highest production volumes in the world. It is estimated that 400 million tons of alkenes are synthesized per year, ethylene being the most predominant olefin in the global market. Platinum is the most active pure metal for light alkane dehydrogenation to produce such alkenes, due to its superior activation of C–H bonds and low activity toward C–C cleavage. However, Pt suffers from a low selectivity, tending to fully dehydrogenate hydrocarbons to pure carbon, leading to coke deposits that block the active sites and deactivate the catalyst. Therefore, even though Pt-based catalysts exhibit high activity in dehydrogenation reactions, the catalyst stability and selectivity are still severe problems in industry.

In this work we studied Pt sub-nanoclusters deposited on MgO(100) for the dehydrogenation of ethane to produce ethylene, using DFT, global optimization techniques, and mechanistic calculations. We performed a computational screening of main-group elements as potential coalloying agents for Pt clusters, with the goal of manipulating the selectivity of catalytic dehydrogenation away from coking. We successfully found a new promising dopant, Si, which stabilizes the clusters against Ostwald ripening (thermal deactivation) and discourages dehydrogenation of ethylene, in comparison to pure Pt clusters. Therefore, Si-doped Pt nanocatalyst are more selective and resistant to deactivation. Si modifies the selectivity of platinum by inducing both electronic and geometric changes, and the effect is persistent across cluster sizes that we considered. Being relatively cheap and naturally abundant, Si constitutes an attractive solution for industry, since it will enable greener and cheaper Pt-based catalysts.



Si-doped Pt clusters are active towards the partial dehydrogenation of ethane, but they exhibit an improved selectivity by halting deeper dehydrogenation, therefore mitigating the deactivation of the catalyst.

Si modifies the selectivity of platinum by inducing both electronic and geometric changes, and the effect is persistent across cluster sizes that we considered. Being relatively cheap and naturally abundant, Si constitutes an attractive solution for industry, since it will enable greener and cheaper Pt-based catalysts.

We emphasize that the results obtained in this work rely on the novel paradigm of theory of cluster catalysis, where an ensemble of accessible catalyst states is considered in property evaluations, instead of just the global minimum structure. Without accounting for alternative isomers thermally populated under conditions of catalysis, the presented effects would not be found.

Observation of topologically protected states at crystalline phase boundaries in single-layer WSe_2

Ugeda MM, Pulkin A, Tang SJ, Ryu H, Wu QS, Zhang Y, Wong D, Pedramrazi Z, Martin-Recio A, Chen Y, Wang F, Shen ZX, Mo SK, Yazyev OV, and Crommie MF.
Nature Communications 9, 3401 (2018)

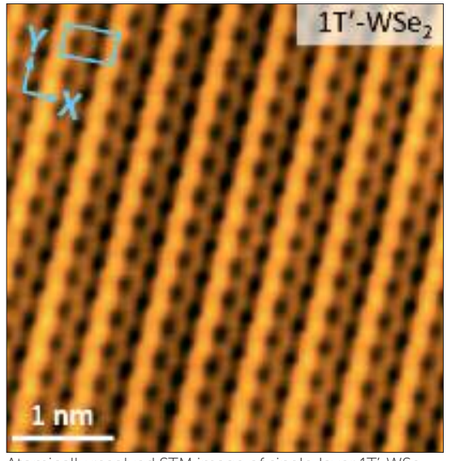
This work presents experimental evidence for the topological quantum spin Hall (QSH) phase with a large bandgap in an isolated, stable two-dimensional (2D) material. Furthermore, we achieve the realization of atomically-precise interfaces with well-ordered topologically-protected edge-states that are directly visualized in real space.

The discovery of the QSH phase in semiconductor quantum wells caused explosive growth in the field of topological materials. While a large number of 3D topological insulators (TI) were subsequently discovered, very few 2D TI are known. Furthermore, these few 2D TI suffer from complex synthesis and/or the need of supporting substrates.

Our work demonstrates that these problems are overcome in a new material system: single-layer 1T'-WSe_2. We show that this single-layer transition metal dichalcogenide (TMD) material is a quantum spin Hall insulator (QSHI) with a large gap (~100meV). We also show that WSe_2 can be phase engineered to exhibit atomically-precise domain boundaries that lead to crystallographically perfect helical edge-states. These edge-states are highly ordered and align with the 2D crystal axes, thus allowing them to be quantitatively analyzed and compared to ab initio theoretical predictions. This verifies the QSH nature of the edge-state that we image using STM spectroscopy, and confirms that this new physical system forms an ideal platform for performing unprecedented quantitative studies of topologically-protected edge modes that exhibit spin-momentum locking.

This represents a significant leap in the field of 2D materials since single-layer 1T'-WSe_2 is a stable QSHI in its isolated, 2D form all the way up to room temperature. This should enable the realization of topology-based 2D flexible devices that exploit dissipationless charge and spin transport. Furthermore, the phase bimorphism of WSe_2 opens the door to new phase engineering of topological-trivial nanostructures that might be exploited in a new generation of QSH-based devices. This creates new opportunities for directly exploring the interplay between different topological states of matter such as QSHIs and 2D superconductors.

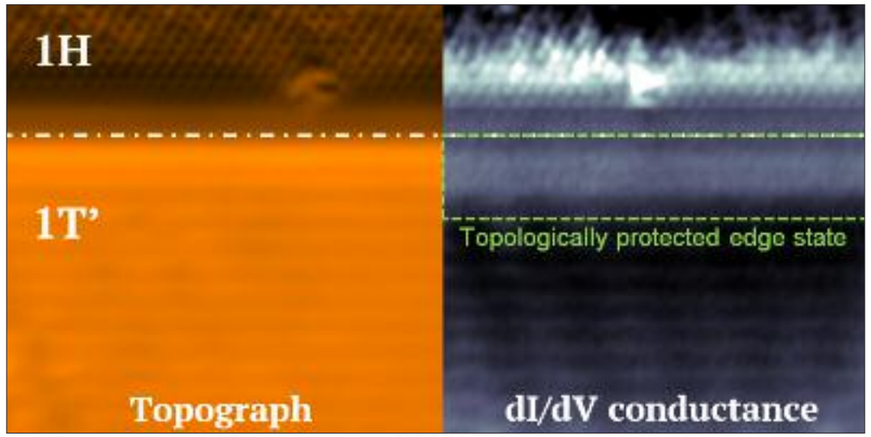
DIPC HIGHLIGHT 2018



Atomically resolved STM image of single-layer 1T'-WSe_2. The unit cell is indicated in blue (V_s=+500 mV, I_t=1 nA).

The single-layer 1T'-WSe_2 system, shown to be a quantum spin Hall insulator, forms an ideal platform for performing unprecedented quantitative studies of topologically-protected edge modes that exhibit spin-momentum locking.

Our work represents a significant leap in the field of 2D materials and may pave the way towards the realization of topology-based 2D flexible devices and a new generation of QSH-based devices.



Left: STM topograph of the 1T'–1H interface (V_s=–525 mV, I_t=0.2 nA).
Right: Experimental dI/dV map of the same area (V_s=–130 meV). White dashed line indicates the 1T'-1H interface, and green dashed lines show the extent of the atomically well-ordered 1D interface state.

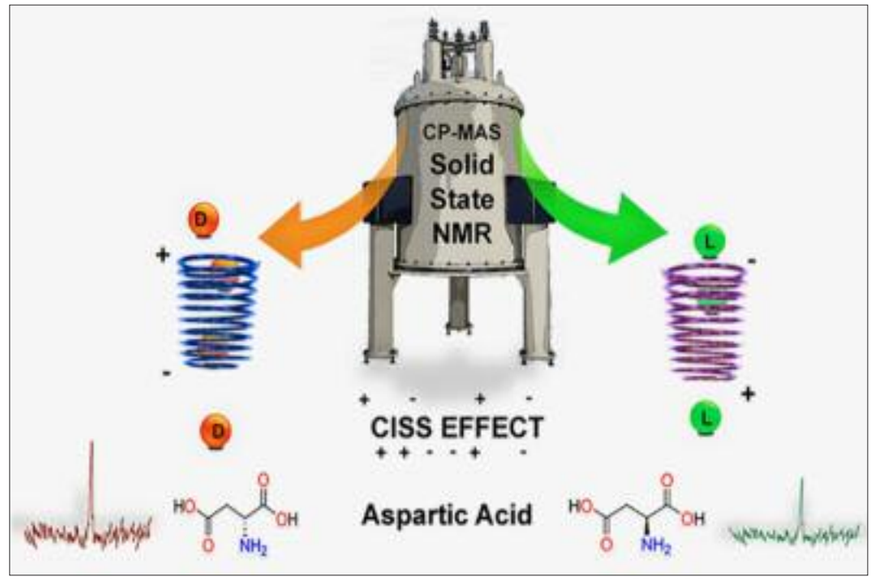
Chirality-induced electron spin polarization and enantiospecific response in solid-state cross-polarization nuclear magnetic resonance

Santos JI, Rivilla I, Cossio FP, Matxain JM, Grzelczak M, Mazinani SKS, Ugalde JM, and Mujica V.
ACS Nano 12, 11426 (2018)

NMR-based techniques are considered to be incapable of distinguishing pure enantiomers; the two mirror images of chiral molecules. In this groundbreaking theory-experiment effort we show that Cross Polarization Solid State NMR produces an enantiospecific response. This unexpected behavior is a hitherto ignored effect of electron spin polarization that breaks the symmetric response of the two enantiomers. The implications of this international effort for the pharmacological and information industries are important.

The serendipitous discovery by the NMR group at UPV/EHU that pure crystalline samples of amino acids can produce an enantiospecific response, triggered a substantial theoretical and experimental international effort to solve this scientific puzzle. The main question that arose from these experiments was: How can an NMR-based technique, contrary to what can be found in all the literature on the subject, distinguish pure optical enantiomers? Finding the answer to this question involved the participation of a team of researchers from the DIPC, the UPV/EHU and Arizona State University. After more than a year of continuous work trying to establish the statistical consistency of the experimental measurements, and the soundness of the theoretical interpretation, our team managed to assemble a manuscript that was recently published in the prestigious ACS Nano journal.

The explanation of the unexpected NMR experiment is ascribed to the subtle electronic spin polarization effect that occurs under the conditions of the Cross Polarization NMR measurement provoking a distinct response for the two enantiomers. This effect, known as Chiral Induced Spin Selectivity (CISS), has been invoked earlier to understand a number of surprising findings in electron transfer, electron transport and bond polarization processes in chiral molecules phenomena.



The center of the figure displays a cartoon-like rendering of the central piece of a CP-MAS Solid State NMR equipment. At the bottom, the molecular structures of the two enantiomers (D and L) of the aspartic acid, and their 1-Hydrogen -15-Nitrogen CP MAS spectra, indicating the same chemical displacement and different intensities for the two enantiomers, which is the main finding of our work. The two enantiomers are also pictorially represented by two helices indicating the different spin polarization pattern (+/-) for each of them.

Chiral molecules, of which amino acids are just one example, are highly relevant in electron transfer processes in biological systems.

The importance of our finding goes beyond its pure scientific relevance. Chiral molecules, of which amino acids are just one example, are highly relevant in electron transfer processes in biological systems. These molecules are optically active, that is they have the property of rotating the plane of polarization of light, and they are present in nature as two enantiomers, which are mirror images of each other. For the pharmacological industry it is of paramount importance to be able to synthesize and certify the enantiomeric purity of samples because often only one of the enantiomers has therapeutic properties while the other is harmful.

Additionally, it does not escape to our attention that the same NMR cross polarization techniques can also be used to transfer spin polarization from the electrons to the nuclei in a lattice, thereby paving the way to the design of molecular architectures that can be used in quantum information.

DIPC HIGHLIGHT 2018

Bioorthogonal catalytic activation of anticancer metal complexes

Alonso-de Castro S, Cortajarena AL, Lopez-Gallego F, and Salassa L.
Angewandte Chemie-International Edition 57, 3143 (2018)

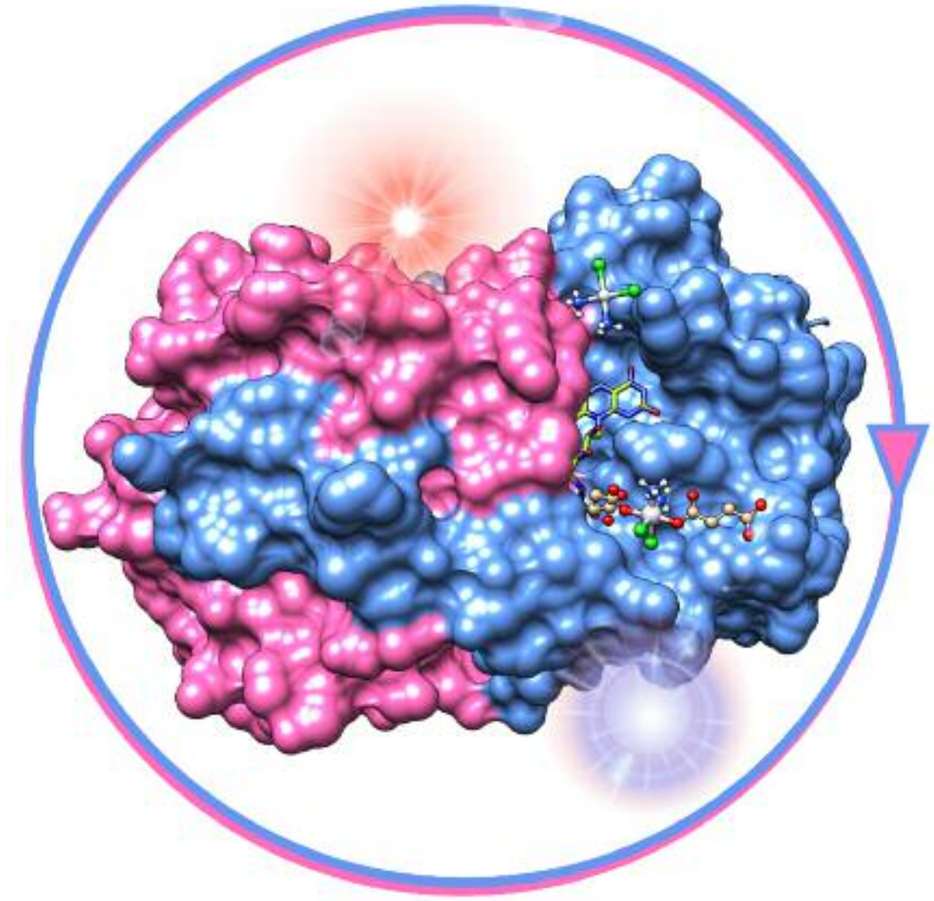
In catalysis, metal complexes are typically regarded as catalysts that convert organic substrates into added value chemicals. In this work, we report a paradigm change in catalysis demonstrating that metal-based anticancer prodrugs can unconventionally act as substrates, and be transformed in their active counterparts by flavoproteins with high efficiency and selectivity.

In cells, flavins are bound to proteins through non-covalent interactions, which control their (photo)redox properties. Our team selected four flavoproteins for their diverse flavin-binding pockets and explored their capacity to prompt the reduction of Pt(IV) prodrugs to Pt(II) cisplatin-like species, both in the dark and under light irradiation. The different chemical environments surrounding the flavin cores of these four flavoproteins control solvent and substrate accessibility to the active site, therefore ruling the efficiency of the catalysis.

Our results show that, in the presence of electron donors and low doses of visible light, the flavoproteins mini singlet oxygen generator (miniSOG) and NADH oxidase (NOX) catalytically activate Pt(IV) prodrugs with bioorthogonal selectivity. In this context, the term bioorthogonal refers to the capacity of a catalytic process to occur selectively with minimal or without unwanted side reactions with biological components. Remarkably, the flavoenzyme NOX also catalyzes Pt(IV) activation in the dark when NADH is the electron donor.

The findings described in this article open new opportunities for the design of chemically and light-activated metal-based chemotherapy drugs, whose biological effects could be triggered endogenously in cells by bioorthogonal flavoprotein catalysts.

The flavoenzyme NOX also catalyzes Pt(IV) activation in the dark when NADH is the electron donor



Coupling of molecular emitters and plasmonic cavities beyond the point-dipole approximation spectroscopy

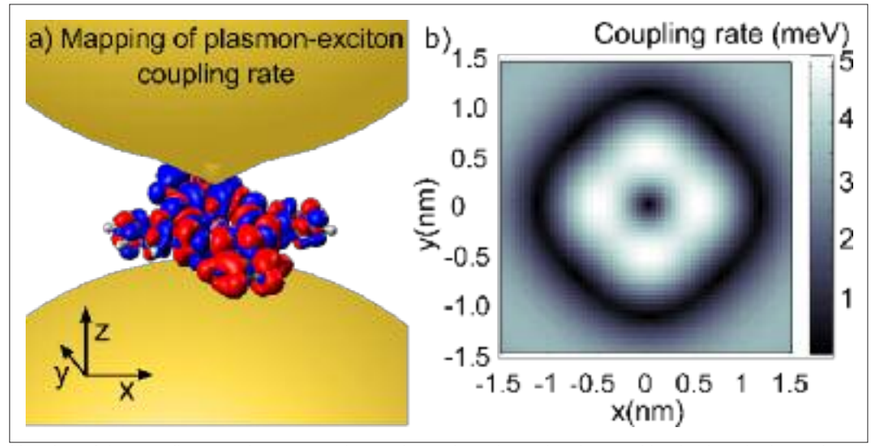
Neuman T, Esteban R, Casanova D, García-Vidal FG, and Aizpurua FJ.
Nano Letters 18, 2358 (2018)

Plasmonic resonances can strongly enhance the strength of the Raman signal emitted by molecules, a considerable advantage for applications that aim at detecting ultra-small quantities. At the same time, however, the plasmon can also distort the signal and thus hide some of the chemical information. This work studies how the photoluminescence signal can be exploited to recover this information.

The interaction between molecular excitons and resonant cavities can be useful for many purposes, including fundamental studies of quantum properties, the detection and characterization of small amount of analyte, or the design of faster on-demand single-photon devices. Metallic nanocavities are very attractive in this context because they support localized plasmons polaritons, resonant oscillations at optical frequencies of the free electron cloud that can localize the electromagnetic energy much beyond the diffraction limit, leading to particularly efficient interaction with the excitons.

Interestingly, the size of the regions of strongest plasmonic fields, called hot-spots, can be as small as ≈1 nanometer, as have been demonstrated, for example, in experiments using Scanning Tunneling Microscope (STM) tips. Under these conditions, the widely used point-dipole approximation, that assumes that the fields are identical at all positions in the molecule, is no longer valid, and new effects can be expected to appear.

This work presents a theoretical framework that goes beyond the point-dipole approximation. We first obtain the spatial distribution of the transition-charge density of a molecular exciton using quantum-chemistry methods based on Time-Dependent Density Functional Theory (TDDFT). In parallel, we decompose the plasmonic response into an infinite number of resonant modes, which are normalized according to the canonical quantization prescription. The Coulomb interaction between the transition-charge density and the charge surface density of each plasmonic mode gives the coupling rates that govern the response.



Mapping of the coupling rates between a plasmonic mode and a molecular transition in zinc phtalocyanine. a) Sketch of the coupling. A molecule is placed between two metallic particles forming a plasmonic cavity. Blue and red colors indicate the transition-charge density corresponding to the molecular exciton under consideration. b) Subnanometrically-resolved map of the coupling rate as the relative position of the molecule and the plasmon in changed. x=y=0 corresponds to the molecule being placed in the center of the cavity

The size of the regions of strongest plasmonic fields, called hot-spots, can be as small as ≈1 nanometer

We use this new framework to study the optical response and exciton dynamics of molecules placed in such extremely confined plasmonic hot-spots. We find significant differences with respect to the point-dipole approximation, including the excitation of transitions that are usually forbidden but that become accessible in our plasmonic system because of the strong field inhomogeneity. This model also naturally demonstrates the possibility of mapping the excitonic response with submolecular resolution and is well suited to study the strong coupling regime, where the plasmon-exciton interaction is so fast that new hybrid modes emerge. Our approach thus allows for more realistic modeling and new insights into the coupling of molecules and plasmonic systems in situations of extreme field localization.

Living nanospear for near-field optical probing

Li YC, Xin HB, Zhang Y, Lei HX, Zhang TH, Ye HP, Saenz JJ, Qiu CW, and Li BJ.
ACS Nano 12, 10703 (2018)

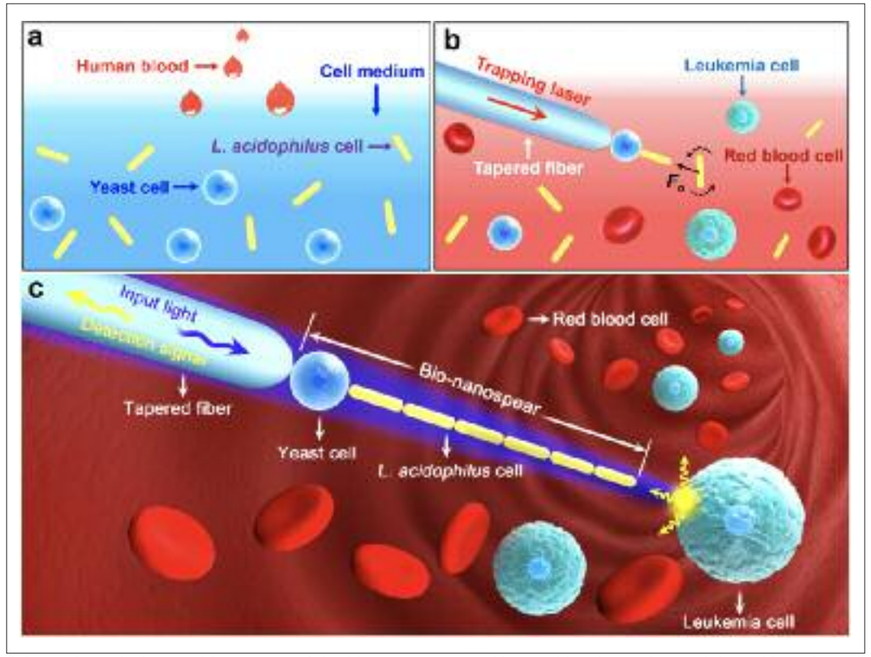
Subwavelength optical probes, designed to emit or collect light in the close proximity of a sample, have been extensively used to image and spectroscopically probe at nanometer resolution. Applications to single-cell manipulation and imaging have triggered an increasing interest in non-invasive probe designs for biomedical applications. However, the available nanoprobes, generally constructed from artificial inorganic materials, are inherently incompatible when interfacing with biological environments.

An ideal nanoprobe would be one that can be made from some biomaterial with appropriate optical properties and soft and flexible enough as not to destroy the specimens. Fortunately, lessons from nature have shown that living cells are native optical materials that possess an amazing ability to manipulate light for their physiological functions. For instance, algae cells are capable of focusing sunlight to improve the efficiency of phototaxis and photosynthesis, and so behave as microlenses. Additionally, living cells in plant stems function as waveguides that can conduct certain wavelengths of light to the roots. Furthermore, Müller cells in human eyes have the capacity to transmit light from the retina surface to photoreceptors, acting as optical fibers. So, why not use some biological cells as optical devices?

Now, an international team of researchers at the Universities of Jinan and Sun Yat-Sen in Guangzhou (China) and NUS (Singapore), including Ikerbasque Research Professor Juan José Sáenz (DIPC), propose a living nanoprobe for near-field probing with subwavelength spatial resolution. The probe is built on a tapered fiber tip apex by optical trapping of a round-shape yeast cell followed by a chain of nanocapsule-shape Lactobacillus acidophilus cells. The spherical yeast cell focuses the trapping laser beam to a nano-jet, which is used to trap the L. acidophilus cells one by one, aligned along the optical axis, forming a high-aspect-ratio telescopic "nanospear".

The proposed bionanospear is flexible and deformable with less chance to puncture and damage the living specimens under measurement, thus it can be used as a noninvasive tool for near-field imaging and sensing of biosamples. The researchers show that light guided through the bio-nanospear can be focused to a subwavelength spot on the surface of a single leukemia cell, demonstrating real-time 190-nm super-resolution imaging of localized fluorescence from the surface of leukemia single-cells in human blood.

With the advantages of its high resolution and biocompatibility, these flexible, non-invasive probes will find important applications in the fields of biosensing and bioimaging.



Schematic optical assembly process of the bio-nanospear. (a) Human blood sample was injected into the cell culture medium of a mixture of yeast and several L. acidophilus cells. (b) A tapered fiber is used to optically trap the yeast cell and several L. acidophilus cells one by one). (c) The bio-nanospear can focus light to a subwavelength spot on the surface of a single leukemia cell.

The proposed bionanospear is flexible and deformable with less chance to puncture and damage the living specimens under measurement

Survival of spin state in magnetic porphyrins contacted by graphene nanoribbons

Li JC, Merino-Diez N, Carbonell-Sanroma E, Vilas-Varela M, de Oteyza DG, Pena D, Corso M, and Pascual JI.
Science Advances 4, eaaq0582 (2018)

Wiring single molecules into electronic circuits requires atomically precise control of their connection to the electrodes. The use of metal electrodes is usually hampered by the lack of well-defined molecule-electrode contacts with high transparency and reproducibility. Graphene and graphene nanoribbons (GNRs) appear as extremely interesting systems for contacting functional molecules via C-C covalent bonds, under the premise that the functionality of the molecules is not affected.

In this frame, synthetic strategies for producing covalent junctions with predefined structures between the molecules and the graphitic leads are crucial. On-surface synthesis, whereby molecules are deposited on a surface that subsequently supports or even drives their covalent coupling, represents an ideal approach for this aim. Its bottom-up nature provides atomic precision that can be controlled by an appropriate design of the molecular reactants, as shown in this work with the creation of well-defined and reproducible hybrid structures comprising porphyrin units as magnetic elements and GNRs as contacting leads. Thus, two types of molecular building blocks are combined: 2,2'-dibromo-9,9'-bianthracene (DBBA in Figure 1a) and Fe-tetra(4-bromophenyl)porphyrin chloride (Br4-FeTPP(Cl) in Figure 1a). The former has been reported to form chiral nanoribbons with edges alternating zig-zag and armchair units in a three to one sequence (i.e. (3,1) cGNRs). The CDH temperature of these ribbons (T≈ 475 K) is relatively low, which reduces the probability of forming by-products. The latter acts as active element, whose Fe ion in the center endows the molecular component with a well-known magnetic ground state. At temperatures slightly above room temperature, the Cl ligand is detached, and the oxidation state of the iron ion changes from Fe+3 to Fe+2. This leaves the Fe-tetraphenyl-porphyrin core (FeTPP in the following) in a S=1 magnetic state. The four Br atoms at the para-phenyl position mediate the covalent connection between FeTPP and GNR via C-C Ullmann coupling reactions, resulting in the polymeric structure shown in Figure 1b. A crucial step for GNR formation is the cyclodehydrogenation reaction. This step creates new C-C bonds, whereby the polymers planarize and form the (3,1) cGNR. We found that CDH also produces an additional 6-membered ring at the FeTPP-cGNR contact (shadowed ring in Figure 1c), which improves the stability and the electronic conjugation of the connection. However, we also observe that the CDH reaction can also affect the porphyrin core by forming new five-membered rings (blue and red arrows in Figure 1c), which fuse the pyrrole moieties to the graphenoid backbone and impose planarity to the tetrapyrrole core. A high-resolution image of a porphyrine coupled to four GNRs is displayed in Figure 1d.

Most importantly, when probed by scanning tunneling spectroscopy, the magnetic properties of contacted porphyrines were maintained, as evidenced with the step-wise increase of conductance at symmetric bias values around the Fermi level that is associated with the inelastic spin excitations of the S=1 spin multiplet. In turn, when probing the contacting GNRs, their electronic properties appeared virtually unperturbed with respect to those of pristine isolated nanoribbons. Thus, on-surface synthesis has been shown to be a viable strategy for incorporating functional molecules into a graphene-based device, while maintaining its functionality.

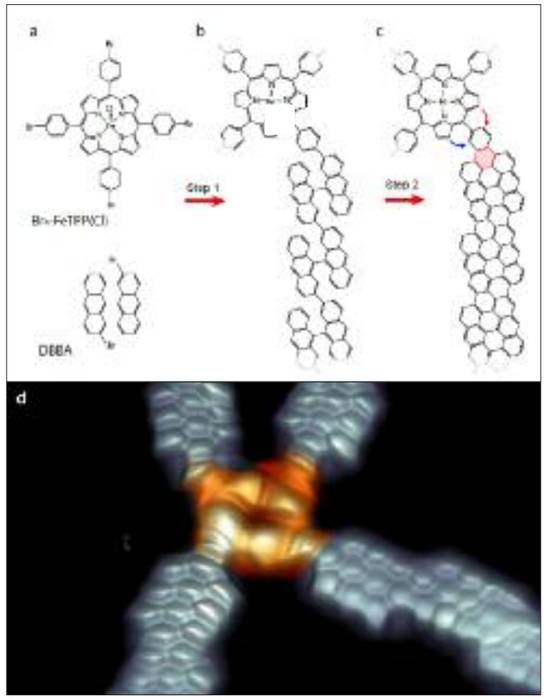


Figure 1. Synthetic strategy for hybrid devices composed of magnetic FeTPP bonded to GNRs. a) Structure of the monomers DBBA and Br4-FeTPP(Cl) (5,10,15,20-Tetrakis-(4-Bromophenyl)-21H,23H-porphine iron(III) chloride) utilized for the on-surface reaction. b) Structure of a hybrid polymer of covalently linked monomers created after the Ullmann coupling step. At the annealing temperatures, the Cl ligand of the porphyrin is detached, whereas the DBBA molecule maintains its three dimensional shape. c) Hybrid device structure after the cyclodehydrogenation (CDH) step. The CDH reaction forms the new ring shadowed red in the image, and can additionally fuse the porphyrin core in a clockwise (red arrow) or anti-clockwise (blue arrow) manner to the contact phenyl. d) High-resolution STM image of a model device structure measured at constant height with a CO-terminated tip.

DIPC HIGHLIGHT 2018

The attosecond streaking with rotating THz field

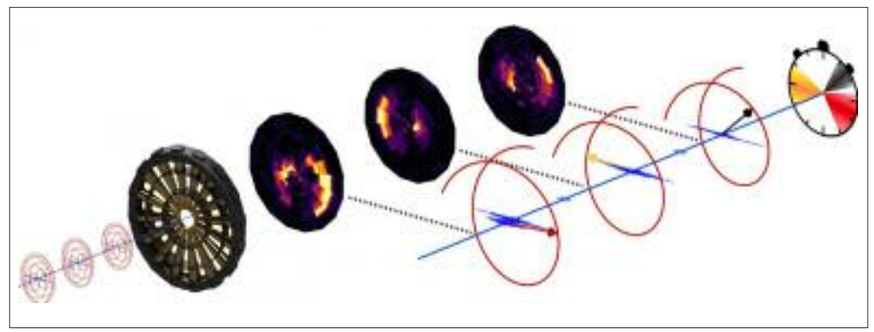
Hartmann N, Hartmann G, Heider R, Wagner MS, Ilchen M, Buck J, Lindahl AO, Benko C, Grunert J, Krzywinski J, Liu J, Lutman AA, Marinelli A, Maxwell T, Miahnahri AA, Moeller SP, Planas M, Robinson J, Kazansky AK, Kabachnik NM, Viefhaus J, Feurer T, Kienberger R, Coffee RN, and Helml W.
Nature Photonics 12, 215 (2018)

Free-electron lasers (FELs) are very prospective experimental tools which generate extremely short and intense X-ray flashes. Researchers hope to use these flashes to resolve structures with diameters on the scale on atomic scale and in time intervals of atomic unit of time, which is about $25{\cdot}10^{-24}$s. However, there is still a principle problem: these pulses are not quite stable from one shot to another, both in the intensity distribution and time duration.

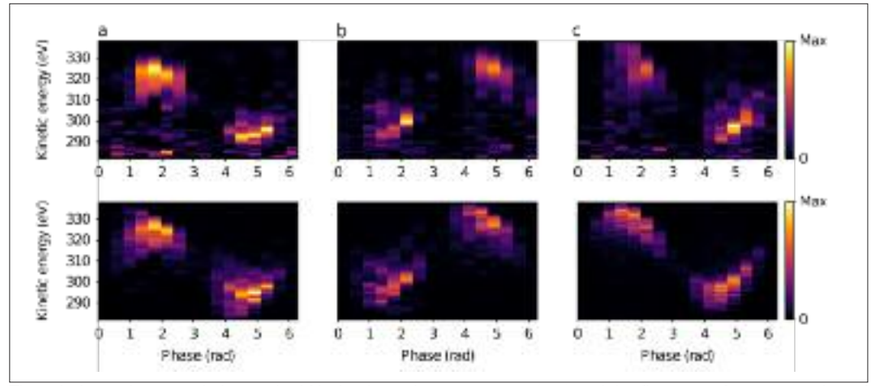
Before FEL pulses can be used to image, for example, biomolecules in extremely high resolution to provide completely new insights into the nano-cosmos of nature, the stable sources and control of the temporal structure of the pulses should be provided. An international team led by physicists at the Technical University of Munich (TUM) has now found a solution: using a circularly polarized infrared laser and a ring of 16 detectors, they can precisely measure the temporal progression and energy of each pulse, making the results obtained from measurements with different pulses comparable. When two such flashes are fired at a sample in rapid succession, information even about the structural changes during a reaction are returned. The first pulse triggers the reaction, while the second laser beam measures changes in the structure caused by the reaction. But the technology has a catch: the temporal progression of the intensity and the duration of the X-ray flashes vary from flash to flash. The results consequently remain blurry.

In their experiment, the research team made the experiments with X-ray flashes from the Linac Coherent Light Source in Menlo Parc (USA). In the sample chamber, they shoot out electrons from neon atoms. If these electrons coincide with an infrared light pulse, they are accelerated or decelerated by its electric field, depending on the field strength of the light pulse when the electron is produced.
The circular polarization of the infrared pulse imparts a direction on the electron, as well. With a ring of 16 detectors, the energy and duration of the original X-ray pulse can be determined with attosecond accuracy as on the dial of a clock.

The theoretical basis of the experiment has been provided by Research Professor from Ikerbasque A.K. Kazansky (DIPC, Donostia, Spain) and by Professor N.M. Kabachnik from Lomonosov State Univeristy (Moscow, Russia).



Initial X-ray pulses ionize the Ne gas target. The external rotating THz field modifies the direction and energy of the ejected electrons in dependence of their ionization time. The X-ray pulses, shown as the shots 1, 2, 3, overlap with the THz pulse at various its phases that leads to the clearly different energy-angle distribution of the ionized electrons. The time-dependence of the X-ray pulse is obtained from scanning the energy-angle distribution of the electrons.



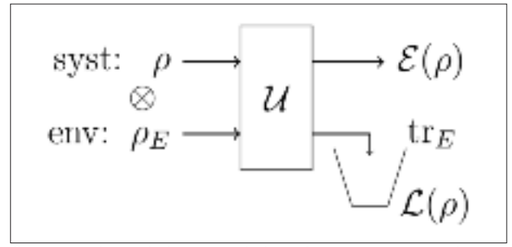
Three independent angularly streaked Ne 1s photoelectron spectra (a-c) and the first step of reconstruction of photoelectron spectra from these data.

DIPC HIGHLIGHT 2018

Degradability of fermionic gaussian channels

Greplova E, and Giedke G.
Physical Review Letters 121, 200501 (2018)

Fermionic quantum channels are a central building block of quantum information processing with fermions, and the family of Gaussian channels, in particular, is relevant in the emerging field of electron quantum optics and its applications for quantum information. Degradable channels are of particular interest since they have a simple formula that characterizes their quantum capacity. We derive a simple standard form for fermionic Gaussian channels, allowing us to fully characterize all degradable n-mode fermionic Gaussian channels.



Quantum channel: the transmission of a quantum state ρ in general involves some processing and inevitable interaction with the environment (in the state ρ_E). These are jointly described by the unitary channel *U*. The channel *E* is obtained by discarding (tracing) the environment. Leakage to the environment is captured by the complementary channel *L* (which describes the signal that, for example, somebody trying to spy on the communication would receive).

Representing and processing information using quantum states offers tremendous advantages in speed and security and is being explored as the basis of a broad range of quantum technologies. A ubiquitous notion in this context are *quantum channels*, which describe the usually imperfect transfer of quantum information in space and time. Nevertheless, noise-free quantum information can be transmitted by employing quantum error correction and using the channel repeatedly. The channel's *quantum capacity* quantifies how many qubits can be transmitted faithfully (in the limit of many channel uses).

Since this quantity involves an optimization over an unlimited number of channel uses, it is typically very hard to compute and only known for very few channels. An important class of channels for which the optimization is tractable are the *degradable* channels. These suffer from a benign (though not necessarily small) form of noise so that the quantum state that leaks to the environment can be reconstructed from the channel output itself.

Mathematically, a quantum channel is represented by *trace-preserving completely positive maps E*. The losses to the environment are described by a second such map, *L*. Now *E* is degradable if and only if there exists a third channel *D* (the "degrading map") that maps the output of *E* to *L, i.e., D·E=L*. While most channels are not degradable, there is no general simple criterion to decide which channels are and which are not. We derive such a criterion for *Gaussian fermionic channels*.

We show that the only degradable such channels correspond to the attenuation or amplitude-damping channel for qubits.

Fermionic quantum channels describe the transmission (or storage) of quantum information encoded in the states of fermions —electrons in semiconductors or superconductors are among the most successful approaches to quantum processors to date—, taking into account the specific statistics of these particles and the superselection rules they obey. Gaussian channels are a simple sub-class that describe *quasi-free* fermions, moving independently, but subject to the effects of their statistics in *phase space*, the space spanned by a set of *modes* that describe the possible single-particle states.

For these channels (on an arbitrary, but finite number of modes) we show that there is only one family of degradable Gaussian fermionic channels. To arrive at the proof, we exploit fermionic phase-space methods. These allow to derive a simple standard form for fermionic channels that simplifies further analysis and allows to give a full characterization of all degradable fermionic Gaussian channels and show that there is only one family of such channels, the single-mode attenuation channel.

This is a channel for which the quantum capacity was already known and thus degradability is not directly useful to compute new quantum capacities. It may be possible to leverage these results to understand bound or estimate the quantum capacity of some approximately-degradable channels or non-Gaussian channels, but further work is required.

DIPC HIGHLIGHT 2018

Bottom-up synthesis of multifunctional nanoporous graphene

Moreno C, Vila-Varela M, Kretz B, Garcia-Lekue A, Costache MV, Paradinas M, Panighel M, Ceballos G, Valenzuela SO, Peña D, and Mugarza A.
Science 360, 199 (2018)

In this work, a novel bottom-up strategy that leads to the formation of atomically precise nanoporous graphene (NPG) is reported. Our combined experimental and theoretical electronic characterization reveals a highly anisotropic electronic structure, where orthogonal one-dimensional electronic bands with an energy gap of ~1eV coexist with confined pore states, making the NPG a highly versatile semiconductor for simultaneous sieving and electrical sensing of molecular species.

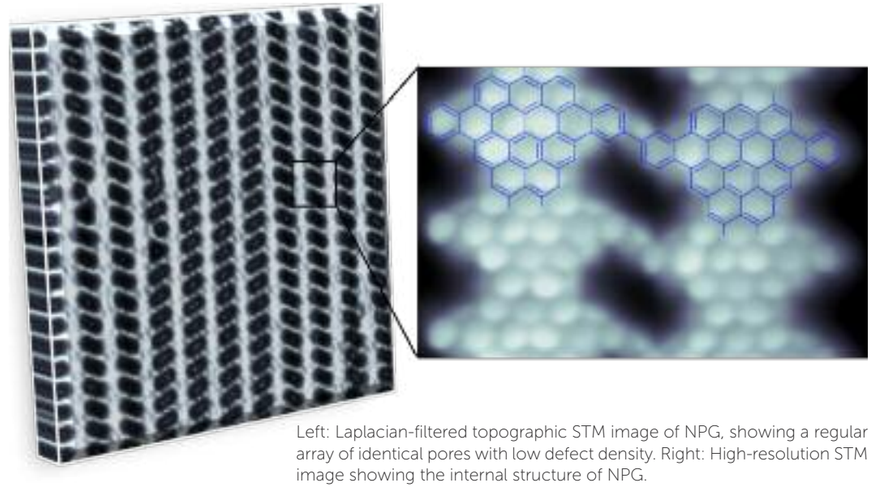
Since the isolation of graphene in 2004, considerable interest has been paid to exploring its application in the field of electronics. But, in order to facilitate the implementation of graphene-based electronic devices, an energy band gap must be opened in its electronic structure. This is possible by patterning an array of closely spaced nanoscopic holes in graphene, thus forming a nanoporous graphene (NPG). Besides, NPG can be much more than an electronic component. It also holds great potential as an atom-thick selective nanosieve for, e.g., DNA sequencing or water purification.

Previous attempts to fabricate NPG relied on top-down approaches, which do not provide atomic scale control of its structure (pore shape/size and distribution). However, combining semiconducting and sieving functionalities in a single NPG material is a challenging task that requires the simultaneous generation of nanometer-sized pores that have to be carved with atomic precision.

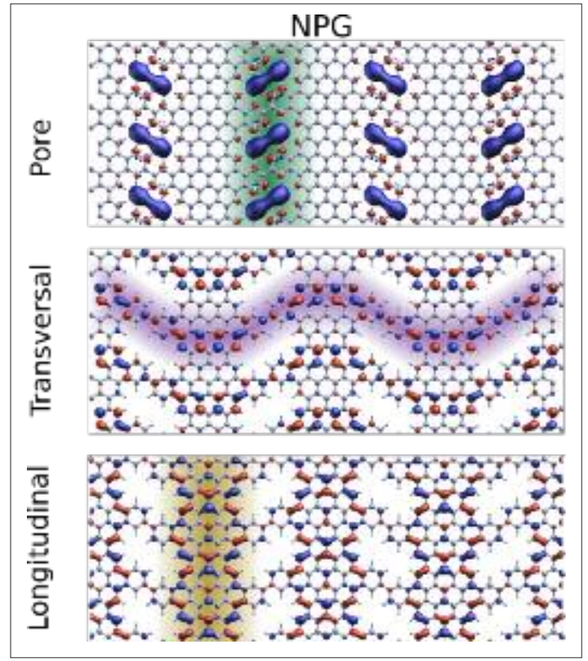
In this work, we report a bottom-up method to synthesize nanoporous graphene comprising an ordered array of pores separated by ribbons, which can be tuned down to the 1-nanometer range. The size, density, morphology, and chemical composition of the pores are defined with atomic precision by the design of the molecular precursors. Combining Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT) a full electronic characterization of this novel 2D material is performed.

We conclude that, the peculiar topology of the NPG imprints a band gap of about ~1eV, one-dimensional (1D) anisotropy and different types of localization in the electronic states, with potential implications in transport and sensing.

The different functionalities of the presented NPG architecture can be exploited in a new generation of graphene-based devices such as FET-sensors, gate-controlled sieves, or chemical and biological sensors and filters. Hence, this study opens numerous avenues for research in different disciplines.



Left: Laplacian-filtered topographic STM image of NPG, showing a regular array of identical pores with low defect density. Right: High-resolution STM image showing the internal structure of NPG.



Examples of calculated longitudinal bands, transversal bands, and localized pore states, highlighted with yellow, purple, and green guiding stripes respectively.

DIPC HIGHLIGHT 2018

Atomic-scale lightning rod effect in plasmonic picocavities: a classical view to a quantum effect

Urbieta M, Barbry M, Zhang Y, Koval P, Sanchez-Portal D, Zabala N, and Aizpurua J.
ACS Nano 12, 585 (2018)

Many of the fascinating properties and applications of plasmonic nanoparticles are based on the ability to enhance and localize the electromagnetic fields down to nanometer scale volumes. The presence of atomic-scale features boosts this localization down to the subnanometric scale, which we explain using a classical model as a nonresonant lightning rod effect at the atomic scale that produces an extra enhancement over that of the plasmonic background.

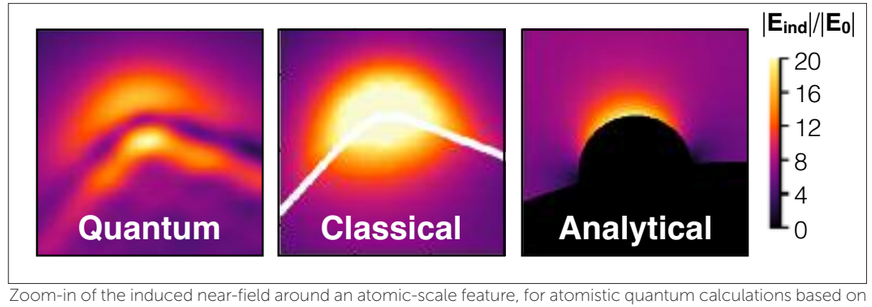
A proper description of the effect of atomic-scale edges, wedges, vertices, and protrusions at surfaces requires a complete quantum theoretical framework, which includes the atomistic structure of the nanoparticles and the wave-like nature of electrons building up the plasmonic excitations. It is important to note that, at the picoscale, the localization of local fields in atomic-scale cavities boosts the coupling of photons with the electronic transitions of single emitters or with the vibrations of a molecule in optomechanical interactions.

Actually, the quantum description of these optical picocavities at the full atomistic level reveals the importance of atomic-scale features. However, such a detailed description is often limited by the computational requirements, even with the relatively efficient time-dependent density functional theory methods.

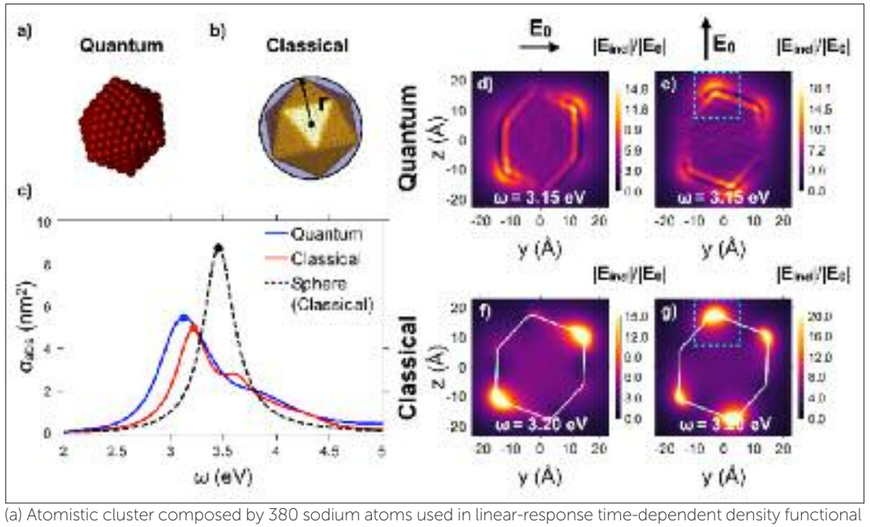
Calculations performed using a boundary element method show that a classical model within the solution of Maxwell's equations, where the atomic-scale features are described by sharp boundaries following the profile of the electron density associated with the atoms, is able to reproduce very satisfactorily the field localization and the effective mode volume in relevant canonical plasmonic nanoresonators such as in single metallic nanoparticles and in nanometric gaps formed by nanoparticle dimers.

A lightning rod effect at the atomic scale is identified as responsible for this extra localization, induced by the electrical potential gradient produced by the electronic wave functions of the atomistic features. When superimposed on top of a nanometric plasmonic resonance, the lightning rod effect acts as a multiplier effect, producing an extra factor of field enhancement, which is characterized by a further spatial localization as compared to the supporting resonance, and a similar spectral distribution.

The existence of picocavities in metallic surfaces has probably been unconsciously revealed in many molecular spectroscopy experiments, enhanced by the action of surface plasmons; however, it is now, with the use of a simplified scheme as shown here, that researchers can start to interpret the effects of atomic-scale features in spectroscopic signals in a compact and simple way by properly addressing the multiscale nature of the hosting cavities.



Zoom-in of the induced near-field around an atomic-scale feature, for atomistic quantum calculations based on linear-response time-dependent density functional theory (LR-TDDFT), calculations within a local classical description using the boundary element method (BEM), and a simplified classical model addressing the multiscale nature of the picocavities.



(a) Atomistic cluster composed by 380 sodium atoms used in linear-response time-dependent density functional theory calculations (LR-TDDFT). (b) Sketch of the continuous icosahedral cluster used for boundary element method (BEM) calculations. The sphere containing the icosahedron has been drawn for reference. (c) Absorption cross section of the particle calculated using LR-TDDFT (blue line) and BEM (red line). The dashed black line corresponds to the absorption cross section of the circumscribing sphere in (b), as calculated with BEM. (d–g) Induced near-field enhancement for a single icosahedral nanoparticle obtained using LR-TDDFT (d, e) and BEM (f, g).

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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

Fellows Gipuzkoa

Dr. Peter Koval
25/11/2013–24/11/2018
Development of MBPT with localized orbitals.

Dr. Aitzol Garcia Etxarri
01/11/2014–Present
Nanophotonics theory.

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. Jorge Sanchez Dolado
02/04/2018–04/07/2018
Thermal and dielectric properties of cement based materials.

Postdoctoral Positions

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

Dr. Joseba Alberdi Rodriguez
01/07/2015–04/01/2018
Morfokinetics: development of computational techniques for the analysis of CVD growth of new 2D materials.

Dr. Marta Pelc
01/12/2015–30/11/2018
Topological defects on carbon like nanostructures.

Dr. Daniel Martinez Tong
11/01/2016–16/12/2018
Local dielectric spectroscopy by AFM. Application to polymer based materials.

Dr. Carlos Garcia Fernandez
20/04/2016–Present
Development of transport methods based on Wannier function.

Dr. Mario Zapata Herrera
01/07/2016–30/04/2018
Quantum and classical approaches to the optical response of metallic nanostructures.

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

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

Dr. Jorge Budagosky Marcilla
01/10/2016–Present
Computational solid state spectroscopy.

Dr. Maxim Ilin
16/12/2016–30/11/2018
Upgrade of MOKE setup to add up the capability for as-susceptibility measurements.

Dr. Beatriz Robles
01/01/2017–31/12/2018
Dynamic properties of concentrated solutions of single chain nanoparticles.

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

Dr. Deung Jang Choi
01/05/2017–31/01/2018
Magnetic states on superconducting surfaces.

Dr. Luciano Colazzo
26/06/2017–25/06/2018
Functional materials synthesized by surface-supported chemistry under vacuum.

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

Dr. Alejandro Rivero Santamaría
09/10/2017–08/10/2018
Dynamics of elementary reactive processes at surfaces.

Dr. Jhon Wilfer Gonzalez Salazar
01/11/2017–31/01/2018
Electronic and magnetic properties of 2D materials and small clusters.

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

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

Dr. Luca Bergamini
01/01/2018–31/07/2018
Optical response of nano-antennas and novel materials.

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

Dr. Macarena Barredo Zuriarrain
05/02/2018–04/08/2018
Generation of 1D/2D/3D optically active nano-microstructures by femtosecond laser induced processing of high quality rare earth doped glasses: spectroscopic characterization and performance.

Dr. Alessio Terenzi
01/03/2018–Present
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. Natalia Koval
01/04/2018–30/11/2018
Ab initio studies on the electronic, elastic and reactive properties of high entropy alloys.

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–Present
Current induced vibrational instabilities in GNR based nanogaps.

Dr. Francesc Monrabal Capilla
01/09/2018–Present
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 Martinez 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 Ibañez
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–Present
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
01/11/2018–Present
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.

PhD Students

Anton Xose Brion Rios
06/02/2013–31/10/2018
Theoretical study on the molecular adsorption and self-organization on substrates of different nature.

Bernhard Kretz
09/06/2014–10/08/2018
Electronic and transport properties of graphenic nanostructures.

Lucía Ortega Álvarez
12/01/2015–10/01/2018
Structure and dynamics of silica filled rubber compounds.

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

Bogusz Bujnowski
01/04/2016–Present
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 Garcia 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–Present
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.

Alvaro Nodar Villa
01/09/2017–30/06/2018
Quantum approaches to the interaction of molecules and plasmonic excitations in nanophotonics.

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

Xabier Telleria Allika
04/09/2017–03/09/2018
Statically screened potentials, Hookean systems and quantum dots.

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

Antton Babaze
01/10/2017–14/01/2018
Quantum approaches to the interaction of molecules and plasmonic excitations in nanophotonics.

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.

Haritz Garai Marin
15/11/2017–30/06/2018
Relaxation of electronic states of magnetic add-atoms at surfaces considering numerical renormalization group (NRG).

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

Mikel Arruabarrena
01/12/2017–31/08/2018
TDDFT approach for the direct calculation of exciton binding energies.

Sebastian Pawel Sitkiewicz
01/01/2018–21/01/2018
Development of density functionals.

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

Garikoitz Aguirregabiria Achutegui
01/02/2018–31/10/2018
TDDFT modelling of the optical response of plasmonics systems.

Mauricio Rodriguez Mayorga
01/02/2018–31/07/2018
Development of improved exchange-correlation functionals.

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–Present
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
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–Present
Electronic correlations and thermalstapility in topological materials.

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

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

Martín Molezuelas
07/11/2018–Present
Quantum Nanophotonics.

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

Technicians

Jordi Torrent Collell
16/06/2018–Present

Silvia Alonso De Castro
01/10–31/12/2018

Alberto Martinez Perez
01/11/2018–Present

Beatriz Romeo Zaragozano
01/11/2018–Present

Daniel Cubero Mimbiela
05/11/2018–Present

Special Assignments

Aran 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

Rubén Esteban
DIPC Summer Internships

Internships

Miguel Blanco Martinez
UPV/EHU, Spain
15/01–06/04/2018
DIPC Computer Center App.

Erik Rodrigues Dopazo
UPV/EHU, Spain
15/01–06/04/2018
Cluster power energy saving system.

Nataliya Nedashkivska
IES Zubiri Manteo, Donostia / San Sebastián, Spain
07/03–18/05/2018
Administración.

José María Caballero Tobajas
UPV/EHU, Spain
21/05–20/07/2018
Installation of a local clould storage system.

Oscar Palomo Iglesias
UPV/EHU, Spain
21/05–20/07/2018
Pilot scheme for micro-computing equipment monitoring.

Maialen Galdeano Fraile
UPV/EHU, Spain
01/06–31/07/2018
Computational study of the reaction mechanism and the role of non-covalent interactions in Frustrated-Lewis pair-based materials.

Josu Salinas Colina
UPV/EHU, Spain
01/06–31/07/2018
Development of open-source computer vision tools for biomedical microscopy data.

Asier Urriolabeitia Rodrigo
UPV/EHU, Spain
01/06–31/07/2018
Molecular dynamics of highly disordered peptides.

Maria Zubiria Ulacia
UPV/EHU, Spain
01/06–31/07/2018
Triplet excitons in PDI derivatives: molecules, dimers and aggregates.

Biel Martinez Diaz
Universidad de Barcelona, Spain
04/06–03/08/2018
Wave packet propagation in graphene nanoribbons.

Eduardo Gónzalez Sánchez
Universidad Autónoma de Madrid, Spain
11/06–20/07/2018
Entanglement transformations of Gaussian fermionic states.

Amaia Juaristi Arrizabalaga
UPV/EHU, Spain
11/06–10/08/2018
Development and theoretical approaches to determine the bond order of graphene-based nanostructures.

Paúl Navarlaz Muguruza
UPV/EHU, Spain
11/06–10/08/2018
Simulation of novel electronic properties in nanostructures.

Celia Gonzalez Sanchez
Universidad Autónoma de Madrid, Spain
15/06–30/06/2018
Exotic magnatism and electron hybridization phenomena in rare earth based materials.

Carmelo Naim
Universitá de Pisa, Italy
18/06–18/08/2018
Good knowledge of quantum chemistry techniques for molecules and their appropriate software.

Asier Zabalo Alonso
UPV/EHU, Spain
25/06–25/08/2018
Topological materials as alloys.

Judit Cizaurre Cuadrado
UPV/EHU, Spain
01/07–31/08/2018
Syntesis and funtionalitation of plasmonic nanocrystals with conjugated polymers.

Alberto Hijano Mendizabal
UPV/EHU, Spain
01/07–31/08/2018
Quantum interference effects due to spin fields in mesoscopic rings.

Iñigo Ansa Isasa
UPV/EHU, Spain
02/07–31/08/2018
Photoactivation of anticancer prodrug systems.

Aritz Dorronsoro Larbide
UPV/EHU, Spain
02/07–31/08/2018
Theoretical study of melting of small metal clusters.

Irati Binue Insausti
Universidad de Deusto, Spain
03/07–31/08/2018
Commumication.

Josep María Armengol Collado
Universitat de Barcelona, Spain
09/07–07/09/2018
Quantum plasmonics.

Mikel Dolz Ruiz
Universidad de Zaragoza, Spain
09/07–08/09/2018
Syntesis of cyclic polymers containing thiol groups.

Urko Lekuona Rico
UPV/EHU, Spain
09/07–31/08/2018
Installation of the advertisement management system in DIPC screens.

Celia Gonzalez Sanchez
Universidad Autónoma de Madrid, Spain
01/09–30/09/2018
Exotic magnatism and electron hybridization phenomena in rare earth based materials.

Adrian Revilla Gomez
UPV/EHU, Spain
01/10–28/12/2018
Improvement of the microinformatics image system.

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).

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. Slawomir Grabowski
01/01/2012–Present
Analyses of intra-and intermolecular interactions in the gas phase, ab initio and DFT calculations as well as the use of the other theoretical methods as for example Quantum theory of atoms in molecules and natural bond orbitals approach. Studies on crystal structures of organic and organometallic compounds, analyses of different Lewis acid.Lewis base interactions (mostly hydrogen bonding) influencing geometries of species constituting crystals and influencing arrangement of molecules and/or ions in crystals, the use of theoretical methods for these analyses as well as statistical methods as for example factor analysis.

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. 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 Garcia 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.

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.

Ikerbasque Research Fellows

Dr. Dario Bercioux
01/10/2014–Present
Quantum transport in nanostructures.

Dr. Rubén Esteban Llorente
01/01/2017–Present
Quantum plasmonics.

Dr. Maia Garcia 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
01/06/2018–Present
Synchrotron researchin superconductors.

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.

Ikerbasque Research Associates

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.

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. David Casanova UPV/EHU
Dr. Miguel Ángel 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
Prof. Francisco José García Vidal UAM
Dr. Miguel Angel Gosalvez UPV/EHU
Dr. Iñaki Juaristi UPV/EHU
Dr. Stefan Kurth UPV/EHU
Dr. Aritz Leonardo UPV/EHU
Dr. Xabier Lopez UPV/EHU
Dr. Nicolás Lorente CSIC
Dr. Jon M. Matxain UPV/EHU
Dr. Jose M. Mercero UPV/EHU
Gabriel Molina Terriza MPC
Dr. Angel Moreno CSIC
Dr. Miguel Moreno Ugeda UPV/EHU
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
Prof. Jesus M. Ugalde UPV/EHU
Prof. Lucia Vitali UPV/EHU
Dr. Nerea Zabala UPV/EHU

Visiting Researchers

Long visits

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

Prof. Miguel Angel Cazalilla Gutierrez
National Tsing Hua University Taiwan, Hsinchu City, Taiwan
05/01/2018–15/02/2018
Spin transport in two dimensional materials.

Dr. Rubén Miguel Ochoa de Zuazola
Hitachi Cambridge Laboratory,
University of Cambridge, UK
01/09/2017–Present
Skyrmions.

Prof. Eugene Kogan
Bar-Ilan University, Ramat-Gan, Israel
16/01–15/04/2018
Graphene vacuum states.

Dr. Chunli Huang
National Tsing Hua University, Hsinchu City, Taiwan
23/11/2017–23/01/2018
Spintronics of low-dimensional materials and interfaces.

Dr. Magdalena Marganska-Lyzniak
Universität Regensburg, Institute for Theoretical Physics, Regensburg, Germany
21/01–25/02/2018
Topological defects in bilayer graphene.

Reece Roberts
Macquarie University, New South Wales, Australia
11/12/2017–11/01/2018
Levitation of nanodiamonds.

Dr. Juan Pablo Echeverry Enciso
Unidad Central del Valle del Cauca, Colombia
31/01–29/04/2018
Dielectric response of 2D layered compounds.

Gaetano Calogero
DTU Nanotech, Technical University of Denmark
15/03–29/04/2018
Large scale simulations of electron trajectories in graphene.

Prof. Juliet Gopinath
University of Colorado Boulder,
Engineering Center ECEE, Colorado, USA
15/03–15/05/2018
Orbital angular momentum in optical fibers combined with plasmonic nanostructures.

Prof. Julian Oberdisse
Laboratoire Charles Coulomb, University of Montpellier, and CNRS, Montpellier, France
31/03–27/04/2018
Structure and dynamics of polymers.

Dr. Svetlana Borisova
Institute of Strength Physics and Materials Science, Siberian Branch of Russian Academy of Sciences, Russian Federation
01/04–30/05/2018
Structure and stability of binary and ternary metallic clusters with strong spin-orbit interaction.

Dr. Galina Rusina
Institute of Strength Physics and Materials Science, Siberian Branch of Russian Academy of Sciences, Tomsk, Russian Federation
01/04–29/06/2018
Phonons in submonolayer structures on metal surfaces.

Prof. Wolfgang Schattke
Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Germany
01/04–31/05/2018
Molecular machines on surfaces:
Nanonmechanical properties of small molecules.

Prof. Oleg Dolgov
Max-Planck Insitut für Festkörperforschung Physics, Stuttgart, Germany
08/04–28/09/2018
Electronic excitations and superconducting instability in solids.

Rafael Muñoz Mármol
Universidad de Alicante, Instituto Universitario de Materiales de Alicante, Spain
09/04–11/05/2018
Simulation of plasmonic systems.

Prof. Christophe Rossel
IBM Research-Zurich, Rüschlikon, Switzerland
09/04–05/05/2018
Electronic properties at the nanoscale oxide electronics perovskites and their applications functional materials.

Prof. Giorgio Benedek
Università degli Studi di Milano-Bicocca, Milano, Italy
17/04–05/06/2018
Electron-phonon interaction theory of inelastic helium atom scattering.

Federica Lumare
Universitá de Pisa, Italy
01/05–31/10/2018
Development of photoactivatable anticancer agents.

Prof. Román Orús Lacort
University of Mainz, Germany
01/05–31/05/2018
Quantum information and condensed matter physics.

Laura Filomena Mazzei
Università Degli Studi di Padova, Italy
03/05–31/07/2018
Development of photoactivatable anticancer agents.

Raúl Amaury Quintero Monsevaiz
CINVESTAV, Ciudad de México, México
07/05–20/12/2018
Open shell PNOF.

Prof. Vladimiro Mújica Hernandez
Arizona State University, USA
25/05–25/08/2018
Chiral-induced spin selecivity effects in molecular environments.

Dr. José Surga Diaz
Instituto Venezolano de Investigaciones Científicas (IVIC), San Antonio de los Altos, Venezuela
28/05–22/08/2018
Atomistics simulations of cement based materials.

Prof. Juan Faustino Aguilera Granja
Instituto de Física de la Universidad Autónoma de San Luis Potosí, México
01/06–31/07/2018
Electronic properties of2-dim nanostructures.

Mikel Iraola Iñurrieta
UPV/EHU, Leioa, Spain
01/06/2018
Analysis of the electronic structure of the strongly correlated compound CuBi2O4 via Group Theory, ab initio methods and Dynamical Mean Field Theory.

Prof. Fernando Martín García
Universidad Autónoma de Madrid, Spain
01/06–31/08/2018
Attosecond dynamics in molecules and surfaces.

Prof. Oleg V. Prezhdo
University of Southern California, Los Angeles, USA
01/06–30/08/2018
Modeling of excitation dynamics in nanoscale materials using time-domain density functional theory and advanced techniques.

Prof. Andrey Vasenko
National Research University Higher School of Economics, Moscow, Russian Federation
01/06–31/08/2018
Anomalous superconductivity and superconductor/ topological insulator proximity effect.

Evan Villafranca
University of Rochester, New York, USA
01/06–01/08/2018
Analysis of entangled photon pair configurations for bright optical sources.

Prof. Carmen Mijangos Ugarte
Consejo Superior de Investigaciones Científicas, Instituto de Ciencia y Tecnología de Polímeros, Madrid, Spain
04/06–03/08/2018
Polymers for nanotecnology. Hierarchical polymer nanostructures.

Prof. Maxim Yu Kagan
P.L. Kapitza Institute for Physical Problems, Russian Academy of Sciences, Moscow, Russian Federation
16/06–15/07/2018
Anomalous superconductivity, Coulomb correlations and electron polaron effect in novel superconductors.

Prof. Pavel Jelínek
Institute of Physics of the Czech Academy of Sciences, Czech Republic
18/06–31/07/2018
Molecules at surfaces.

Prof. Erik Diaz Cervantes
Universidad de Guanajuato, Tierra Blanca, México
25/06–23/07/2018
Design of 2D-materials based on GaAs.

Ane Aguirre Gonzalez
01/07–30/09/2018
Computational engineering of hydrogenase enzymes.

Prof. Miguel Angel Cazalilla Gutierrez
National Tsing Hua University Taiwan, Hsinchu City, Taiwan
01/07–31/08/2018
Spin transport in two dimensional materials.

Prof. Sergey Eremeev
Institute of Strength Physics and Materials Science, Tomsk, Russian Federation
01/07–31/07/2018
Electronic structure of topological insulators.

Prof. Javier Garcia de Abajo
ICFO-Instituto de Ciencias Fotonicas, Castelldefels, Barcelona, Spain
01/07–31/07/2018
Plasmons in ultrathin metal films. Surface Science to nano-optics and plasmonics

Prof. Francisco José Garcia Vidal
Facultad de Ciencias, Universidad Autónoma de Madrid, Spain
01/07–31/07/2018
Polaritonic photovoltaics

Prof. Francisco Guinea López
Imdea Nanoscience, Madrid, Spain
01/07–31/07/2018
Theory of two dimensional materials

Prof. Maria Angeles Hernandez Vozmediano
Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain
01/07–31/07/2018
Topological matter.

Prof. Nikolay Kabachnik
Institute of Nuclear Physics, Moscow State University, Russian Federation
01/07–30/09/2018
Theoretical study of short pusle induced Auger processes in atoms.

Prof. Luis Martin Moreno
Instituto de Física de Materiales de Aragón, Universidad de Zaragoza, Spain
01/07–31/07/2018
Theory on nanophotonics.

Dr. Miguel Martinez Canales
The University of Edinburgh, School of Physics & Astronomy, Edinburgh, UK
01/07–31/07/2018
Properties of metallic alloys at earth's core conditions. Implementing Raman spectrum calculations in espresso for PBE.

Dr. Tatiana Menshchikova
Tomsk State University, Tomsk, Russian Federation
01/07–28/09/2018
Investigation of the electronic structure of topological insulators using first-principles calculations.

Prof. Talat Shahnaz Rahman
University of Central Florida, UCF, Orlando, USA
01/07–31/07/2018
Theoretical and computational investigations of transport, magnetic and optical properties of functional nanomaterials.

Dr. Igor Rusinov
Tomsk State University, Tomsk, Russian Federation
01/07–28/09/2018
Investigation of the Weyl semimetal, topologically non trivial systems using first-principles and model calculations.

Prof. Daniel Loss
University of Basel, Switzerland
06/07–05/08/2018
Quantum transport in nanostructures.

Prof. Gabriel Cwilich
Yeshiva University, New York, USA
15/07–10/08/2018
Random media, quantum optics.

Prof. Richard Korytár
Charles University, Prague, Czech Republic
15/07–15/08/2018
Transport signatures of overlapping Kondo clouds in a coherent Kondo lattice formed in magnetic adatoms on a surface of a metal. Slave-boson mean-field approximation.

Prof. Pablo Artal Soriano
Universidad de Murcia. Spain
24/07–23/08/2018
Biomedical optics.

Dr. Unai Atxitia
Freie Universität Berlin, Germany
01/08–31/08/2018
Theoretical investigation of possible sub-picosecond spin switching nanoscale antiferromagnets.

Dr. Roman Kuzian
Institute for Problems of Materials Science National Academy of Sciences of Ukraine, Kiev, Ukraine
01/08–31/10/2018
Photoemission from strongly correlated systems.

Prof. Vladimir Kuznetsov
National Research Tomsk State University, Tomsk, Russian Federation
01/08–31/08/2018
Topological insulators.

Prof. Gernot Frenking
Philipps-Universität Marburg, Germany
06/08–30/11/2018
Quantum theory of the chemical bond.

Dr. Chun Li Huang
The University of Texas at Austin, USA
09/08–09/09/2018
Spin transport in two-dimensional materials.

Prof. Peter Gill
Research School of Chemistry, Australian National University, Canberra, Australia
12/08–11/09/2018
Study of intracule functions of the pair density.

Efrem Bernuz Conill
Universitat de Barcelona, Spain
01/09–30/09/2018
Implement a set of features and modules to SYMEESS software to calculare continuous measures of shape and symmetry of molecules.

Maria Zubiria Ulacia
UPV/EHU, Donostia / San Sebastián, Spain
01/09–31/10/2018
Triplet states in PDI and related organic molecules.

Prof. Ceferino Lopez Fernandez
Instituto de Ciencia de Materiales (CSIC), Madrid, Spain
07/09–06/10/2018
Disorder photonics.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
16/09–31/10/2018
Electron-phonon interaction theory of inelastic helium atom scattering.

Prof. Vladimir Menshov
National Research Centre, Kurchatov Institute, Moscow, Russian Federation
16/09–15/12/2018
QAHE in heterostructures topological insulator / magnetic normal insulator.

Prof. Mariona Sodupe Roure
Universidad de Barcelona, Cerdanyola del Valles, Spain
16/09–15/10/2018
Quantum chemistry of peptides involved in neorudegenerative deceases.

Prof. Joseph Richard Manson
Clemson University, Clemson, South Carolina, USA
24/09–31/10/2018
Electron-phonon interactions near surfaces.

Prof. Julio A. Alonso Martín
Facultad de Ciencias, Universidad de Valladolid, Spain
01/10–31/10/2018
Interaction between molecules and supported nanoparticles.

Prof. Anna Krylov
University of Southern California, Los Angeles, USA
01/10–31/10/2018
Solar energy; quantum chemistry methods.

Prof. Amand Lucas
University of Namur, Belgium
02/10–31/10/2018
Surface physics.

Prof. Raffaele Resta
Instituto Officina dei Materiali, CNR, Trieste, Italy
02/10–05/12/2018
Geometrical and topological properties of the electronic ground state.

Prof. Marijan Sunjic
University of Zagreb, Croatia
02/10–31/10/2018
Electronic structure and energy transfer processes in graphene.

Prof. Godfrey Gumbs
Hunter College, City University of New York, USA
03/10–31/10/2018
Charge Fractionalization without electron-electron interaction in bilayer silicene.

Prof. Vladimir Nazarov
Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan
06/10–05/11/2018
Quantum-mechanical description of the inelastic scattering of low-energy electrons.

Alejandra Granja del Río
Facultad de Ciencias, Universidad de Valladolid, Spain
28/10–28/11/2018
Ab initio molecular dynamics of H2 on Pd clusters supported on graphene.

Prof. Michael Rappaport
Weizmann Institute o Science, Faculty of Physics, Rehovot, Israel
15/09–15/12/2018
PETALO

Dr. Jacek Generowicz
CERN, Meyrin, Switzerland
01/10–30/11/2018
PETALO

Short visits

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
11/12/2017–06/01/2018
Electronic and structural properties of low dimensional systems.

Prof. Godfrey Gumbs
Hunter College, City University of New York, USA
08/01–02/02/2018
Coulomb excitations of black phosphorus and bismuth-based heterostructures.

Prof. Liliana Arrachea
Universidad de Buenos Aires, Argentina
09/01–12/01/2018
Quantum energy transport and thermoelectrics in driven systems.

Dr. Edwin van Der Heide
Leiden University, Netherlands
10/01–10/01/2018
Questions in art and science.

Dr. María José Calderón Prieto
Instituto de Ciencia de Materiales de Madrid (CSIC) Madrid, Spain
11/01–12/01/2018
Silicon based quantum computing

Prof. Nate Bastian
Astrophysics Research Institute, Liverpool John Moores University, UK
14/01–16/01/2018

Dr. Stefano A. Mezzasalma
Ruder Boskovic Institute, Laboratory for Optics and Optical Thin Films, Zagreb, Croacia
14/01–19/01/2018
Light-driven self-assembly of plamonic nanoparticles.

Dr. Alexander Riss
Technische Universität München, Germany
14/01–21/01/2018
Bond-resolving non-contact atomic force microscopy applied to on-surface synthesis.

Dr. Pablo Lopez Tarifa
VU University - Faculty of Sciences, Amsterdam, Netherlands
15/01–18/01/2018
SIESTA development: improvements in real-time TDDFT.

Prof. Zaher Salman
Paul Scherrer Institut, Villigen, Switzerland
15/01–19/01/2018
Topological materials and heterostructures.

Dr. Pascal Larregaray
Institut des Sciences Moléculaires, Université de Bordeaux, France
17/01–19/01/2018
Ab-initio methods for studying the physics and chemistry of adsorption processes at surfaces.

Dr. Anika Schlenhoff
Institute of Nanostructure- and Solid State Physics, University of Hamburg, Germany
24/01–26/01/2018
Image potential states on magnetic materials.

Prof. Juan Ignacio Cirac
Max-Planck-Institut für Quantenoptik, Garching, Germany
25/01–26/01/2018
New frontiers in quantum optics and quantum information.

Dr. Thi Nga Do
National Kaohsiung Normal University, Kaohsiung city, Taiwan
26/01–02/02/2018
Defect-enriched electronic properties of group-IV 2D systems.

Po Hsin Shih
National Cheng Kung University, Tainan City, Taiwan
26/01–02/02/2018
Defect-enriched electronic properties of group-IV 2D systems.

Dr. Carlos Sanchez Cano
University of Warwick, UK
26/01–26/01/2018
Studying the secret life of organometallic complexes inside cells.

Dr. Aires Lemos Gonçalves Ferreira
University of York, UK
31/01–02/02/2018
Proximity-induced skew scattering: a new mechanism for spin Hall effect

Prof. Itziar Laka Mugarza
Universidad del País Vasco (UPV/EHU), Vitoria-Gazteiz, Spain
01/02–02/02/2018
Presentación película "Arrival"

Prof. Marijan Sunjic
University of Zagreb, Croatia
01/02–27/02/2018
Dynamical response and surface excitations in thin films.

Prof. Ricardo Amils Pibernat
Centro de Astrobiología, CSIC-INTA, asociado al Instituto de Astrobiología de la NASA, Torrejón de Ardoz, Spain
16/02–17/02/2018
The dark biosphere, gemicrobiology of the subsurface of the Iberian Pyrite Belt.

Kateryna Domina
V. N. Karazin Kharkiv National University, Kharkiv, Ukraine
16/02–28/02/2018
Plasmonics in ferromagnetic nanostructures.

Dr. Liubov Ivzhenko
IRE of NASU, Kharkov, Ukraine
16/02–28/02/2018
Plasmonics in ferromagnetic nanostructures.

Prof. Sara Russell
National History Museum, London, UK
16/02–17/02/2018
Meteorites: unlocking the secrets of our origin

Dr. Pablo Lopez Tarifa
VU University - Faculty of Sciences, Amsterdam, Netherlands
19/02–23/02/2018
SIESTA development: improvements in real-time TDDFT.

Prof. Zaher Salman
Paul Scherrer Institut, Villigen, Switzerland
20/02–23/02/2018
Topological materials and heterostructures.

Dr. Rafael Rebolo López
Instituto de Astrofísica de Canarias, Santa Cruz de Tenerife, Spain
21/02–23/02/2018
Astrophysics.

Dr. Kevin Vynck
LP2N (Laboratoire Photonique Numérique et Nanosciences), Institut d'Optique d'Aquitaine, Talence, France
25/02–27/02/2018
Light propagation in disordered correlated media.

Dr. Gavin Brennen
Macquarie University, Australia
27/02–28/02/2018
Quantum attacks on bitcoin.

Prof. Emi Minamitani
Graduate School of Engineering, University of Tokyo, Bunkyo-ku, Tokyo, Japan
04/03–10/03/2018
Atomic scale investigation of low-energy excitation at surface and interface by inelastic electron tunneling spectroscopy.

Prof. Elisa Jimenez Izal
University of California, Los Angeles, USA
08/03–09/03/2018
Computational materials chemistry: Design of heterogeneous nanocatalysts and two-dimensional materials.

Dr. Bruce Milne
Universidade de Coimbra, Portugal
11/03–19/03/2018
Predicting properties of biogenic materials with machine learning.

Prof. Luis Alberto Montero Cabrera
Universidad de La Habana, Cuba
11/03–27/03/2018
Understanding singlet fission as a photonic enhancing effect.

Prof. Robert M. Westervelt
Harvard University, John A. Paulson School of Engineering and Applied Sciences, Cambridge, Massachussetts, USA
11/03–19/03/2018
Integrated quantum materials.

Prof. Andrey Varykhalov
Helmholtz-Zentrum Berlin, Synchrotron BESSY II, Berlin, Germany
12/03–14/03/2018
Unoccupied scaterring resonances in graphene.

Dr. Victor Escobedo Bermudez
Christian-Albrechts-Universität zu Kiel, Germany
13/03–14/03/2018
Literature and science.

Dr. Laura Morrón Ruiz de Gordejuela
Next Door Publishers, Pamplona, Spain
14/03–15/03/2018
Literature and science.

Prof. Mads Brandbyge
DTU Nanotech, Technical University of Denmark, Lyngby, Denmark
15/03–22/03/2018
Large scale simulations of electron trajectories in graphene.

Dr. Chen Chen
University of California at Berkeley, USA
15/03–15/03/2018
Characterizing and manipulating electronic structures of on-surface synthesized nano-materials.

Prof. Rafael Marcos Yuste Rojas
The NeuroTechnology Center at Columbia University, Biological Sciences, New York, USA
17/03–25/03/2018
Neurophysics.

Prof. Juan Faustino Aguilera Granja
Instituto de Física de la Universidad Autónoma de San Luis Potosí, México
18/03–07/04/2018
Electronic properties of nanostructures (tubes, and bencen rings).

Dr. Joshua Renner
Universidad de Valencia, Valencia
18/03–23/03/2018
Experimental particle physics.

Prof. Javier Garcia de Abajo
Surface Science to nano-optics and plasmonic-sICFO-Instituto de Ciencias Fotonicas, Castelldefels, Barcelona, Spain
19/03–20/03/2018
Surface science to nano-optics and plasmonics.

Friedrich Maass
University of Heidelberg, Heidelberg, Germany
20/03–23/03/2018
2D-Plasmon at metal/organic interfaces.

Prof. Annemarie Pucci
Heidelberg University, Heidelberg, Germany
20/03–23/03/2018
Low dimensional plasmonic excitations on surfaces.

Prof. Petra Tegeder
Heidelberg University, Physical Chemistry Institute, Heidelberg, Germany
20/03–24/03/2018
Low dimensional plasmonic excitations on surfaces.

Dr. Paula Natalia Abufager
Instituto de Física Rosario, Rosario, Argentina
08/04–06/05/2018
Electronic and transport properties at the nanoscale.

Prof. Nate Bastian
Astrophysics Research Institute, Liverpool John Moores University, UK
11/04–15/04/2018
Astrophysics.

Dr. Raúl Angulo
Centro de Estudios de Física del Cosmos de Aragón, CEFCA,Teruel, Spain
12/04–14/04/2018
Numerical simulations in cosmology.

Dr. Barry Bradlyn
Princeton University, New Jersey, USA
15/04–05/05/2018
Topological photonic crystals.

Guadalupe Ruiz
Universitat Politécnica de Catalunya, Barcelona, Spain
15/04–18/04/2018
Hydrated prilocaine in confined systems.

Prof. Pablo Artal Soriano
Laboratoria de Optica, Universidad de Murcia, Spain
18/04–19/04/2018
Physics for a better vision.

Dr. Roberto Robles Rodríguez
ICN2, Barcelona, Spain
19/04–20/04/2018
Spin-orbit coupling studies of materials: some examples.

Miguel Bello
Instituto de Ciencia de Materiales del CSIC, Madrid, Spain
22/04–24/04/2018
Nuclear spins in quantum dots.

Prof. Erik B. Berda
University of New Hampshire, Durham, USA
22/04–27/04/2018
Synthesis and characterization of single-chain nanoparticles.

Prof. Salvador Miret Artes
CSIC, Instituto de Física Fundamental, Madrid, Spain
22/04–26/04/2018
Theory of surface diffusion.

Prof. Gloria Platero
Instituto de Ciencia de Materiales del CSIC, Madrid, Spain
22/04–24/04/2018
Modeling and simulation of materials.

Prof. Claudia Felser
Max Planck Institute for Chemical Physics of Solids, Dresden, Germany
26/04/0208–02/05/2018
Spintronics meeting.

Prof. Stuart Parkin
Max Planck Institute of Microstructure Physics, Halle, Germany
26/04–02/05/2018
Spintronics meeting

Dr. György Hantal
Computational Physics Group, Faculty of Physics, University of Vienna, Austria
03/05–04/05/2018
Intrinsic analysis of instantaneous fluid interfaces in computer simulations.

Prof. Garnett Bryant
National Institute of Standards and Technology, NIST, Gaithersburg, MD, USA
06/05–13/05/2018
Quantum plasmonics.

Prof. Emily Townsend
NIST/Joint Quantum Institute/ University of Maryland, USA
06/05–13/05/2018
Quantum plasmonics.

Dr. Aurora Nogales Ruiz
Instituto de Estructura de la Materia CSIC, Madrid, Spain
07/05–08/05/2018
Applications of Dielectric Spectroscopy to study soft matter phase transitions in real time.

Prof. Augusto Beléndez Vázquez
Universidad de Alicante, San Vicente del Raspeig, Alicante, Spain
10/05–12/05/2018
Maxwell and the electromagnetic theory of light.

Prof. Predarg Lazic
Rudjer Boskovic Institute, Zagreb, Croatia
16/05–24/05/2018
Research topic: ab initio calculations of intercalation of graphene on metals.

Dr. Ivor Loncaric
Rudjer Boskovic Institute, Zagreb, Croatia
16/05–24/05/2018
Theoretical methods to study femtosecond laser desorption processes.

Dr. Dino Novko
Institute of Physics (Center of Excellence for Advanced Materials and Sensing Devices), Zagreb, Croatia
16/05–24/05/2018
Vibrational lifetime of adsorbates on surfaces.

Dr. Tom Broadhurst
UPV/EHU, Spain
17/05–18/05/2018
New dark waves from the cosmos: Bose-Einstein interference vs. primordial black holes.

Prof. Angel Fernandez Recuero
Jot Down
18/05–19/05/2018
Colaboration with Jot Down

Prof. Guy Le Lay
Aix-Marseille Université, Marseille, France
21/05–15/06/2018
Silicene.

Prof. Fabio Donati
IBS Center for Quantum Nanoscience, Seoul, Republic of Korea
24/05–30/05/2018
Spin excitations in rare earth elements on MgO.

Prof. Julio Lloret Fillol
Institut Català d'Investigació Química (ICIQ), Tarragona, Spain
24/05–25/05/2018
Towards light-driven reduction. from solar fuels to solar chemicals.

Lorenzo Monacelli
Universitá di Rome La Sapienza, Italy
25/05–25/06/2018
Theoretical study of the high pressure phase diagram of hydrogen.

Prof. Naomi Halas
Rice University, Houston, Texas, USA
29/05–01/06/2018
Plasmonics: from stained glass to sustainability and societal impact.

Prof. Tristan Cren
Institut des NanoSciences de Paris, CNRS & UPMC, Paris, France
30/05–02/06/2018
Topological superconductors and majorana fermions

Prof. Gilberto Teobaldi
Stephenson Institute for Renewable Energy, The University of Liverpool, UK
31/05–02/06/2018
Between Scylla and Charybdis (by density functional theory): fundamental challenges, opportunities and advances in functional interfaces.

Guzmán Lopez Espejo
Universidad de Málaga, Spain
01/06–22/06/2018
Thermally activated delayed fluorescence in triptycene derivatives.

Fani Madzharova
Humboldt-Universität zu Berlin, Germany
04/06–29/06/2018
Plasmon-enhanced second harmonic generation from core-shell nanostructures.

Dr. Yuan Zhang
Aarhus University, Denmark
05/06–10/06/2018
SERS from molecules in plasmonic nano-cavities.

James Lawrence
University of Warwick, Coventry, UK
06/06–08/06/2018
On-surface synthesis of functional materials.

Prof. Ingmar Swart
Utrecht University, Utrecht, Netherlands
07/06–09/06/2018
Lattice systems with integer pseudo-spin.

Roberto Constantini
CNR-IOM, Trieste, Italia
09/06–30/06/2018
STM imaging on 1,4,9,10-Tetrahydroxy-anthracene molecules

Prof. Luis Alberto Montero Cabrera
Universidad de La Habana, La Habana, Cuba
09/06–24/06/2018
Machine learning applied to predict molecular spectra.

Prof. Valentin Freilikher
Bar-Ilan Uiversity, Ramat-Gan, Israel
10/06–03/07/2018
Light propagation in disordered media.

Prof. Christian Schöenenberger
University of Basel, Switzerland
14/06–15/06/2018
Cooper-pairs are nice, but split ones too!

Prof. Vasily Stolyarov
Moscow Institute of Physics and Technology (State University) (MIPT), Russian Federation
24/06–27/06/2018
Strong spin-orbit coupling in topological insulator systems.

Prof. Ulrich Höfer
Philipps-Universität Marburg, Fachbereich Physik, Marburg, Germany
26/06–04/07/2018
Structure and fynamics of internal interfaces.

Prof. Alexander Golubov
University of Twente, Enschede, Netherlands
27/06–04/07/2018
Electronic excitations and superconducting nstability in solids.

Rishav Harsh
Université Paris-Diderot, Laboratoire Matériaux et Phénomènes Quantiques, Paris, France
29/06–09/07/2018
Donor-acceptor molecular assemblies on graphene/SiC(0001).

Dr. Roland Hayn
Institut Materiaux Microelectronique Nanosciences de Provence, Faculté des Sciences et Techniques, Marseille, France
01/07–07/07/2018
Spin-resolved GW for solid state systems.

Prof. Jorge Kohanoff
School of Mathematics and Physics, Queen's University Belfast, Northern Ireland, UK
04/07–22/07/2018
Dynamical simulation of irradiation processes.

Prof. Daniel Granados Ruiz
IMDEA Nanociencia. Madrid, Spain
05/07–05/07/2018
Playing old physics with new materials: From PN junctions to Light-Matter interactions

Prof. Roberto Raimondi
Roma Tre University, Italy
09/07–14/07/2018
Investigation of spin-orbit coupling effects in the charge and spin properties of metals and semiconductors.

Diego Romero Abujetas
Instituto de Estructura de la Materia, IEM-CSIC, Madrid, Spain
09/07–12/07/2018
Theory of light scattering in nano-structured highly refractive media.

Prof. José Manuel Pereira Carmelo
Universidade do Braga, Portugal
16/07–30/07/2018
Correlated quantum systems.

Dr. Maxim Kharitonov
Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany
20/07–03/08/2018
Bulk boundary correspondence in topological media.

Dr. Dmitri Efremov
IFW Dresden Researcher, Dresden, Germany
23/07–29/07/2018
Electronic excitations and superconducting instability in solids.

Prof. Antonio Miguel Garcia Garcia
Shanghai Jiao Tong University, Shanghai
01/08–04/08/2018
Interplay of disorder and superconductivity in 2D materials.

Dr. Francisco Kitaura Joyanes
IAC, ULL, La Laguna, Santa Cruz de Tenerife, Spain
06/08–15/08/2018
Computational cosmology.

Prof. José Nelson Onuchic
Center for Theoretical Biological Physics (CTBP) Rice University, Houston, USA
13/08–16/08/2018
Exploring the energy landscape for protein folding and function: the convergences of structural models and sequence coevolution information.

Dr. Sergio Contreras Hantke
Centro de Estudios de Física del Cosmos de Aragón (CEFCA), Teruel, Spain
15/08–18/08/2018
Computational cosmology.

Prof. Nicolas Regnault
CNRS - ENS París, France
22/08–24/08/2018
Topological materials.

Dr. Barry Bradlyn
Princeton University, New Jersey, USA
24/08–27/08/2018
Topological photonic crystals.

Prof. Oliver Hahn
Laboratoire Lagrange, Observatoire de la Côte d'Azur, Nice, France
26/08–01/09/2018
Dark matter modelling, Large-scale structure.

Dr. Munisai Nuermaimaiti
Graduate School of Science, Hiroshima University, Japan
26/08–01/09/2018
Topological Insulators

Ifeanyi John Onuorah
Universitá di Parma, Italy
26/08–09/09/2018
Anharmonic effects for muons.

Susanne Schulz
TU, Technische Universität Dresden, Germany
26/08–02/09/2018
Bulk and surface electronic properties of rare-earth compounds.

Xiaoxiao Wang
Hiroshima University, Japan
26/08–01/09/2018
Topological insulators.

Dr. Mao Ye
Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai, China
26/08–30/08/2018
Topological insulators.

Prof. Akio Kimura
Hiroshima University, Japan
27/08–01/09/2018
Topological insulators.

Dr. Sivan Refaely-Abarmson
University of California, Berkeley; Lawrence Berkeley National Laboratory, USA and Weizmann Institute of Science, Israel
29/08–31/08/2018
First-principles DFT-based methods applied to complex and correlated systems.

Prof. Fernando Quevedo
Abdus Salam International Centre for Theoretical Physics, ICTP, Trieste, Italy
01/09–03/09/2018
High energy physics.

Dr. Stefano A. Mezzasalma
Ruder Boskovic Institute, Laboratory for Optics and Optical Thin Films, Zagreb, Croatia
02/09–14/09/2018
Shape-dependent optical properties of plasmonic nanoparticles. Experiments vs theory.

Prof. Andrey Borissov
Institute of Melecular Science in Orsay, CNRS, Université París-Sud, Orsay Cedex, France
05/09–08/09/2018
Quantum plasmonics.

Prof. Andreas Heinrich
Center for Quantum Nano Science, Institute for Basic Science, Ehwa Womans University, Republic of Korea
05/09–09/09/2018
Quantum nanoscience: atoms on surface.

Prof. Ulrich Honenester
University of Graz, Austria
06/09–09/09/2018
Electron energy losses and nanophotonics.

Prof. Dudley Herschbach
University of Harvard, Cambridge, Massachusetts, USA
08/09–10/09/2018

Dr. Cosimo Gorini
Universität Regensburg, Germany
10/09–13/09/2018
Magneto-transport in (shaped) topological insulator nanowires.

Dr. Hender Lopez Silva
University of Tübingen, Germany and Institute Laue-Langevin, Grenoble, France
10/09–15/09/2018
Simulations of hydrodynamics in polymeric nanoparticles.

Dr. Sergio Contreras Hantke
CEFCA, Centro de Estudios de Física del Cosmos de Aragón, Teruel, Spain
12/09–15/09/2018
Computational cosmology.

Dr. Mark Neyrinck
Universidad del País Vasco, UPV/EHU, Bilbao, Spain
13/09–14/09/2018
Cosmic web.

Prof. Cesar Aurelio Herreño Fierro
Universidad Distrital Francisco José de Caldas, Bogotá, Colombia
14/09–18/09/2018
Magnetoplasmonics.

Kristen Kaasbjerg
Technical University of Denmark, Denmark
14/09–14/09/2018
Unprecedented transport properties of monolayer TMD devices: experiment and theory.

Prof. Wlodzimierz Jaskólski
Nicolaus Copernicus University, Faculty of Physics, Astronomy and Informatics, Torun, Poland
16/09–30/09/2018
Spin-resolved topological states in defectd bilayer graphene.

Prof. Fabrizio Dolcini
Politecnico di Torino, Torino, Italy
17/09–30/09/2018
Mesoscopic Physics

Prof. Alessandro De Martino
University of London, UK
24/09–03/10/2018
Effects of spin-orbit coupling on transport properties of graphene pn-junctions.

Prof. Arnaud Desmedt
Institut des Sciences Moléculaires, Université de Bordeaux I, France
24/09–25/09/2018
Dynamics of clathrates hydrates.

David Izquierdo Villalba
CEFCA, Centro de Física del Cosmos de Aragón, Teruel, Spain
24/09–05/10/2018
Work on model of galaxy formation and black hole evolution.

Prof. François Englert
Université Libre de Bruxelles, Belgium
25/09–04/10/2018
Reconstructing the Universe

Dr. Juan José García Ripoll
IFF, CSIC Madrid, Spain
26/09–29/09/2018
Quantum computing and quantum simulation with superconducting circuits.

Dr. Magdalena Marganska-Lyzniak
Universität Regensburg, Institute for Theoretical Physics, Regensburg, Germany
30/09–21/10/2018
Topological states at lattice defects in bilayer graphene.

Dr. Paloma Arroyo Huidrobo
Imperial College London, UK
01/10–02/10/2018
Symmetries in plasmonic systems: from metasurfaces to topological phases of light.

Prof. Michael Berry
Bristol University, UK
02/10–07/10/2018
Superresolution waves.

Prof. Archie Howie
Cavendish Laboratory,
University of Cambridge, UK
02/10–16/10/2018
Comparison of photonics and fast electron interactions for plasmonics.

Tetiana Rokhmanova
Kharkiv National University, Ukraine
02/10–02/10/2018
Photonics with bulk and surface electromagnetic waves in layered superconductors.

Daria Sostina
Paul Scherrer Institut, Villigen, Switzerland
02/10–06/10/2018
Molecule-matal interfaces.

Prof. Gerardus t'Hooft
Institute for Theoretical Physics, Utrecht, Netherlands
02/10–06/10/2018
Quantum black hole physics.

Prof. Frank Pollmann
Technical University of Munich, Germany
04/10–04/10/2018
Novel phases of matter in strongly interacting systems.

Dr. Joanna Page
University of Cambridge, UK
10/10–11/10/2018
Tomás Saraceno: The art and science of cosmopolitics.

Kateryna Domina
V. N. Karazin Kharkiv National University, Kharkiv, Ukraine
12/10–03/11/2018
Magnetic-field controlable optical lensing.

Prof. Salvador Miret Artes
CSIC, Instituto de Física Fundamental, Madrid, Spain
14/10–18/10/2018
Electron phonon coupling.

Luis Enrique Aguilar Suarez
Zernike Institute for Advanced Materials, Faculty of Science and Engineering, University of Groningen, Groningen, Netherlands
15/10–18/10/2018
Theoretical study of the singlet fission process.

Dr. Claudia Climent Biescas
Facultad de Ciencias, Universidad Autónoma de Madrid, Spain
15/10/2018
Polaritonic photophysics and photochemistry.

Philipp Schmoll
University of Mainz, Germany
15/10–30/10/2018
Non-abelian symmetries in tensor network algorithms.

Prof. Shirin Faraji
Zernike Institute for Advanced Materials, Faculty of Science and Engineering, University of Groningen, Groningen, Netherlands
15/10–18/10/2018
Theoretical study of the singlet fission process.

Prof. Christophe Rossel
IBM Research-Zurich, Rüschlikon, Switzerland
19/10–22/10/2018
Electronic properties at the nanoscale oxide electronics - perovskites and their applications functional materials.

Dr. Shy Genel
Flatiron Institute, New York, USA
21/10–23/10/2018
Galaxy formation seminar

Dr. Carlos Hernandez Monteagudo
CEFCA, Teruél, Spain
24/10–26/10/2018
BACCO, cosmology.

Mairi Sakellariadou
King's College London, UK
26/10–30/10/2018
Science does not get along with make-dos, like models: it needs theories.

Prof. Francisco Gonzalez Fernandez
Facultad de Filosofía y Letras,
Universidad de Oviedo, Spain
30/10–31/10/2018
Poincaré en la orilla: observaciones sobre la invención científica.

James Lawrence
University of Warwick, UK
05/11–30/11/2018
Functional materials synthesized by surface supported chemistry under vacuum.

Prof. Norio Okabayashi
Kanazawa University, Japan
05/11–13/11/2018
Investigation of inelastic electron tunneling process.

Dr. Juan Bermejo Vega
FU Berlin, Dahlem Center for Complex Quantum Systems, Berlin, Germany
07/11–13/11/2018
Quantum computing and quantum simulation.

Dr. Federico Di Paolo
Instituto Volcanológico de Canarias - INVOLCAN, Tenerife, Spain
08/11–10/11/2018
Radar evidence of subglacial liquid water on Mars

Johannes Knörzer
MPI für Quantenoptik, Garching, Germany
11/11–25/11/2018
Quantum acoustics.

Prof. Javier Garcia de Abajo
ICFO-Instituto de Ciencias Fotonicas,
Castelldefels, Barcelona, Spain
13/11–14/11/2018
Surface science to nano-optics and plasmonics.

Prof. Thomas Ebbesen
ISIS, Université de Strasbourg & CNRS, Strasbourg, France
14/11–17/11/2018
The Alchemy of Vacuum – Hybridizing Light and Matter

Prof. Kai Rossnagel
Kiel University / DESY Hamburg, Kiel, Germany
14/11–18/11/2018
Time-resolved photoemission spectroscopy at free-electron lasers.

David Izquierdo Villalba
Centro de Física del Cosmos de Aragón (CEFCA), Teruel, Spain
18/11–30/11/2018
Work on model of galaxy formation and black hole evolution.

Daniele Spinoso
Centro de Física del Cosmos de Aragón (CEFCA), Teruel, Spain
18/11–30/11/2018
Models of black hole formation.

Prof. Guang Ye
Delft University of Technology, Delft, Netherlands
27/11–29/11/2018
Multi-scale transport modelling and its application to the service life prediction of concrete structures

Dr. Martin Zeleny
Institute of Material Science and Engineering, Brno University of Technology, Czech Republic
29/11–01/12/2018
Stability of nanotwinned martensitic structures in Ni-Mn-Ga magnetic shape memory alloys.

Prof. Guinievere Kauffmann
Max Planck Institute for Astrophysics, München, Germany
09/12–15/12/2018
Cosmology and structure formation.

Prof. Timur Shegai
Chalmers University of Technology, Göteborg, Sweden
09/12–11/12/2018
Light emission in hybrid nanostructures.

Jens Stucker
Max Planck Institute for Astrophysics, München, Germany
09/12–15/12/2018
Warm dark matter simulations.

Prof. Simon White
Max Planck Institute for Astrophysics, München, Germany
09/12–15/12/2018
Cosmology and structure formation.

Prof. Stephen Hughes
Queen's University, Engineering Physics & Astronomy, Kingston, Canada
12/12–15/12/2018
Nanophotonics.

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

Dr. Juan Carlos Idrobo Tapia
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Tennessee, USA
16/12–20/12/2018
Temperature dependence of electron energy loss spectroscopy.

Dr. Pierre François Loos
CNRS, Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier, Toulouse, France
16/12–18/12/2018
Reduced density matrix functional theory.

Maria Tenorio
Institut Català de Nanociència i Nanotecnologia, Barcelona, Spain
17/12–21/12/2018
Ab-initio electronic properties of nanoporous graphene.

Personnel

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Luz Fernández
Operation and Help Desk Manager

Diego Lasa
Computing Services Manager

Daniel Franco
HPC Resources Technician

Seminars

1 Selected CI and Jastrow-free QMC methods for Chemistry
17/12/2018
Pierre-Francois Loos
CNRS Universite Paul Sabatier, Toulouse, France

2 Plasmon — exciton interactions at a single nanoantenna level
10/12/2018
Timur Shegai
Department of Physics, Chalmers University of Technology, Göteborg, Sweden

3 Stability of nanotwinned martensitic structures in Ni-Mn-Ga magnetic shape memory alloys
30/11/2018
Martin Zeleny
Brno University of Technology, Czech Republic

4 Multi-scale transport modelling and its application to the service life prediction of concrete structures
29/11/2018
Guang Ye
Delft University of Technology, Delft, Netherlands

5 Geometrical observables of the electronic ground state
23/11/2018
Raffaele Resta
Istituto Officina dei Materiali, CNR, Trieste, Italy

6 Taming electrons with surface waves: acoustic and magnetic traps for electrons in semiconductors
22/11/2018
Johannes Knoerzer
Max-Planck Institute for Quantum Optics, Garching, Germany

7 Time-resolved photoemission spectroscopy at free-electron lasers
16/11/2018
Kai Rossnagel
Kiel University and DESY, Germany

8 Travelling in Valence Space
14/11/2018
Gernot Frenking
Fachbereich Chemie, Philipps-Universität, Hans-Meerwein-Strasse, Marburg, Germany

9 Radar evidence of subglacial liquid water on Mars
09/11/2018
Federico Di Paolo
Instituto Volcanológico de Canarias - INVOLCAN, Tenerife, Spain

10 Outperforming classical computers with near-term quantum devices: a new optic
08/11/2018
Juan Bermejo Vega
Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany

11 Investigation of inelastic electron tunneling process by combining STM and AFM
07/11/2018
Norio Okabayashi
Kanazawa University, Japan

12 Poincaré en la orilla: observaciones sobre la invención científica
31/10/2018
Francisco González Fernández
Universidad de Oviedo, Spain

13 Tackling strong correlation: Spin-flip method and its applications to single molecular magnets
26/10/2018
Anna I. Krylov
University of Southern California, USA

14 Galaxy Formation and galaxy morphologies with modern cosmological hydrodynamical simulations
22/10/2018
Shy Genel
Center for Computational Astrophysics, New York, USA

15 Cavity-modified ground-state chemical reactivity
19/10/2018
Clàudia Climent Biescas
Universidad Autónoma de Madrid, Spain

16 Tomás Saraceno: The art and science of cosmopolitics
11/10/2018
Joanna Page
University of Cambridge, UK

17 Topological electronic states in metal-coordinated organic networks
05/10/2018
Daria Sostina
University of Basel, Switzerland

18 Novel Phases of matter in strongly interacting systems
04/10/2018
Frank Pollmann
Technical University of Munich, Germany

19 Photonics with bulk and surface electromagnetic waves in layered superconductors
02/10/2018
Tetiana Rokhmanova
Kharkiv National University, Ukraine

20 Proximity-induced superconductivity in Landau-quantized graphene monolayers
28/09/2018
Alessandro De Martino
University of London, UK

21 Ultrastrong coupling with propagating photons
27/09/2018
Juan García-Ripoll
IFF, CSIC, Madrid, Spain

22 Developing models for chromatin folding
14/09/2018
Jose Onuchic
Rice University, Texas, USA

23 Unprecedented transport properties of monolayer TMD devices: Experiment and theory
14/09/2018
Kristen Kaasbjerg
Technical University of Denmark (DTU), Kongens Lyngby, Denmark

24 Magneto-transport in (shaped) topological insulator nanowires
11/09/2018
Cosimo Gorini
Universität Regensburg, Germany

25 New Ways to think about electronic excited states
10/09/2018
Peter Gill
Australian National University, Canberra, Australia

26 Complex Excitonic phenomena in photophysics from advanced computational approaches
30/08/2018
Sivan Refaely-Abarmson
University of California, Berkeley; Lawrence Berkeley National Laboratory, USA

27 Spin-dependent Chemistry
27/07/2018
Vladimiro Mujica
Arizona State University, School of Molecular Sciences, USA

28 Effect of disorder in multi-band superconductors
25/07/2018
Dmitri Efremov
Leibnitz Institute for Solid State Physics and Material Science IFW-Dresden

29 New anomaly induced transport in 3D Dirac matter
13/07/2018
Maria Angeles Hernandez Vozmediano
ICMM-CSIC, Madrid, Spain

30 Metal-organic spin chains by on-surface polymerization
06/07/2018
Roland Hayn
Institut Materiaux Microelectronique Nanosciences de Provence, Faculté des Sciences et Techniques, Marseille, France

31 Playing old physics with new materials: From PN junctions to Light-Matter interactions
05/07/2018
Daniel Granados
IMDEA Nanociencia, Madrid, Spain

32 Recent developments in time-domain coupled-cluster theory for quantum chemistry
29/06/2018
Daniel Nascimento
Georgia Institute of Technology - School of Chemistry and Biochemistry, USA

33 A view of science in Cuba by a Cuban scientist in the global 21st. Century scenario
22/06/2018
Luis Alberto Montero Cabrera
Universidad de La Habana, Cuba

34 Novel exotic forms of low-dimensional epitaxial Si, Ge, and Sn: silicene, its cousins, and related Xenes
13/06/2018
Guy Le Lay
PIIM-CNRS, Aix-Marseille University, France

35 Designing Quantum Matter: fabrication and characterization with atomic scale precision
08/06/2018
Prof. Ingmar Swart
Utrecht University, Netherlands

36 Attochemistry: imaging and controlling electron dynamics in molecules with attosecond light pulses
07/06/2018
Prof. Fernando Martín
Universidad Autónoma de Madrid and IMDEA Nano, Spain

37 On-surface self-assembly, reactions and electronic properties of PXX and binol derivatives
07/06/2018
James Lawrence
University of Warwick, Coventry, UK

38 Between Scylla and Charybdis (by Density Functional Theory): fundamental challenges, opportunities and advances in functional interfaces
01/06/2018
Prof. Gilberto Teobaldi
Stephenson Institute for Renewable Energy, The University of Liverpool, UK

39 Topological superconductivity in 1D and 2D systems
31/05/2018
Dr. Tristan Cren
Institut des NanoSciences de Paris, CNRS & UPMC, Paris, France

40 Spin dynamics of Ho single atom magnets
25/05/2018
Fabio Donati
IBS Center for Quantum Nanoscience, Seoul, Republic of Korea

41 Towards light-driven reduction. From solar fuels to solar chemicals
25/05/2018
Julio Lloret
Institut Català d'Investigació Química (ICIQ), Tarragona, Spain

42 New Dark waves from the cosmos: bose-einstein interference vs. primordial black holes
18/05/2018
Tom Broadhurst
Ikerbasque, UPV/EHU, Donostia / San Sebastián, Spain

43 2D van der Waals materials and some new aspects of surface science
17/05/2018
Prof.Predrag Lazic
Rudjer Boskovic Institute, Zagreb, Croatia

44 Maxwell y la teoría electromagnética de la luz
11/05/2018
Prof.Augusto Beléndez Vázquez
Universidad de Alicante, San Vicente del Raspeig, Alicante, Spain

45 Applications of Dielectric Spectroscopy to study soft matter phase transitions in real time
08/05/2018
Dr. Aurora Nogales Ruiz
Instituto de Estructura de la Materia CSIC, Madrid, Spain

46 Atom-based photonics, quantum plasmonics and many-body physics
07/05/2018
Prof. Garnett Bryant
National Institute of Standards and Technology, NIST, Gaithersburg, MD, USA

47 Intrinsic analysis of instantaneous fluid interfaces in computer simulations
04/05/2018
Dr. György Hantal
Computational Physics Group, Faculty of Physics, University of Vienna, Austria

48 Language is renormalization (and its implications in physics, linguistics and machine learning)
03/05/2018
Roman Orus
Johannes Gutenberg-Universität Mainz, Germany

49 Topological Materials with liquid electrons
27/04/2018
Claudia Felser
Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

50 Long range transport in ac-driven quantum dot arrays
24/04/2018
Prof. Gloria Platero
Department of Theory, Modeling and Simulation of Materials Instituto de Ciencia de Materiales del CSIC, Madrid, Spain

51 Spin-orbit coupling studies of materials: some examples
20/04/2018
Dr. Roberto Robles
Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain

52 Physics for a better vision
19/04/2018
Pablo Artal
Laboratorio de Óptica de la Universidad de Murcia, Spain

53 Generation and detection of tunable orbital angular momentum in polarization-maintaining optical fiber
17/04/2018
Juliet T. Gopinath
Department of Electrical, Computer and Energy Engineering, University of Colorado at Boulder, USA

54 The E-MOSAICS project: simulating the formation and evolution of galaxies and their globular cluster systems across full cosmic history
13/04/2018
Prof. Nate Bastian
Astrophysics Research Institute, Liverpool John Moores University, UK

55 Science and Technology center for integrated quantum materials
16/03/2018
Prof. Robert M. Westervelt
Harvard University, Massachusetts, USA

56 Computational materials chemistry: Design of heterogeneous nanocatalysts and two-dimensional materials
09/03/2018
Prof. Elisa Jimenez Izal
Department of Chemistry and Biochemistry, University of California, Los Angeles, USA

57 Atomic scale investigation of low-energy excitation at surface and interface by inelastic electron tunneling spectroscopy
05/03/2018
Prof. Emi Minamitani
University of Tokyo, Japan

58 Quantum attacks on bitcoin
27/02/2018
Gavin Brennen
Macquarie University, Australia

59 Poor man's scaling: Kondo and Coqblin-Schrieffer models
23/02/2018
Prof. Eugene Kogan
Bar-Ilan University, Ramat-Gan, Israel

60 Meteorites: unlocking the secrets of our origin
16/02/2018
Prof.Sara Russell
National History Museum, London, UK

61 The dark biosphere, gemicrobilogy of the subsurface of the Iberian Pyrite Belt
16/02/2018
Prof. Ricardo Amils Pibernat
Centro de Astrobiología (associate of the NASA Astrobiology Institute), CSIC-INTA, Spain

62 Studying the secret life of organometallic complexes inside cells
26/01/2018
Dr.Carlos Sanchez-Cano
University of Warwick, UK

63 Image potential states on magnetic materials
25/01/2018
Anika Schlenhoff
Institute of Nanostructure- and Solid State Physics, University of Hamburg, Germany

64 Neutrinos and medical imaging: the odd couple or (another) example of how fundamental physics is tied to our daily life.
19/01/2018
Dr. Paola Ferrario
Ikerbasque, DIPC, Donostia / San Sebastián, Spain

65 Materials Science at the Atomic Scale: Structure, chemical reactions and complex architectures
18/01/2018
Dr. Alexander Riss
Technische Universität München, Germany

66 Thermal Behavior of nanolattices co-deposited with an oxide matrix
17/01/2018
Dr. Stefano A. Mezzasalma
Ruder Boskovic Institute, Laboratory for Optics and Optical Thin Films, Zagreb, Croatia

67 Silicon based quantum computing
12/01/2018
Dr. María José Calderón
Instituto de Ciencia de Materiales de Madrid (CSIC) Madrid, Spain

68 Quantum energy transport and thermoelectrics in driven systems
11/01/2018
Prof. Liliana Arrachea
Universidad de Buenos Aires, Argentina

69 Questions in Art and Science
10/01/2018
Dr. Edwin van der Heide
Leiden University, Netherlands

Workshops

Light Magnetoelectric Effects on nanostructures (LIMAGE) 142

ImagineNano 2018 143

Functional Polymers 147

International Spring School on High Performance Computing 148

Euskal Esperientziak Zientzia Zabalkuntzan (EEZZ18) 150

Novel 2D materials explored via scanning probe microscopy & spectroscopy 152

Single Atom Ba Tagging (SABAT) 154

Quantum Designer Physics 156

New Generation in Strongly Correlated Electrons Systems (NGSCES 2018) 158

Spins on Surfaces (SoS II) 160

Theoretical Methods in Molecular Spintronics 162

On-Surface Synthesis International Workshop (OSS-18) 164

XIII International Ontology Congress 166

Spanish Conference on Nanophotonics (CEN2018) 168

HOPDSS2018 170

Transborder QuantumChemPhys Lab Workshop 172

From Bioinorganic Chemistry to Catalysis 174

Software Carpentry 176

Light Magnetoelectric Effects on Nanostructures (LIMAGE)

February 7-9, 2018
DIPC, Donostia / San Sebastián
http://limage2018.dipc.org/

Organizers
J.A. Sánchez-Gil (IEM-CSIC, Madrid)
J.J. Sáenz (DIPC, Donostia /San Sebastián)

The aim of the workshop was to review the state of the art and new trends in the theoretical understanding and experimental investigation of the interaction of electromagnetic fields with nanostructured matter.

In the spirit of DIPC Workshops, LIMAGE provided a friendly atmosphere to foster discussions and collaborations in particular between emergent and more experienced scientists in the field of light-matter interactions, by encouraging participation of PhD students and researchers at an early stage of their career. For this purpose, the program of the conference included contributions of selected speakers as well as oral presentations by PhD students and PostDocs chosen among the contributed abstracts.

Topics included:
❖ Light-Matter angular momentum transfer.
❖ Optical binding and sorting.
❖ Near-field and evanescent wave interactions.
❖ Optical trapping in photovoltaics.
❖ Nanowire and Nanoparticle photonics.
❖ Nanooptics and nanostructured devices.

Invited Speakers
J. Aizpurua (CFM-CSIC
P. Albella (ULPGC)
C. Aragó (UAM)
R. Delgado-Buscalioni (IFIMACUAM)
Rubén Esteban (DIPC)
A. García-Etxarri (DIPC)
A. García-Martín (IMN-CSIC)
V. Giannini (IEM-CSIC)
F. González (UC)
R. Hilenbrand (CIC nanoGUNE)
D. Jaque (UAM)
L. Liz-Marzán (BioMagune)
M.I. Marqués (IFIMAC-UAM)
G. Molina-Terriza (CFM-CSIC)
F. Moreno (UC)
M. Nieto-Vesperinas (ICMM-CSIC)

ImagineNano 2018

March 13-15, 2018
Bilbao Exhibition Centre (BEC), Bilbao
http://www.imaginenano.com/2018/

Organizing Committee
Phantoms Foundation (Bilbao)
DIPC (Donostia / San Sebastián)

Bilbao (Spain) was the host of the 4th edition of the largest European Event in Nanoscience & Nanotechnology. Following the overwhelming success of Imagine-Nano 2015 (www.imaginenano.com), several conferences were held in parallel, as well as a vast exhibition (free entrance to professionals after online registration), one-to-one meetings and an industrial forum. ImagineNano gathered the global nanotechnology community, including researchers, industry policymakers and investors.

Plenary Speakers
Avelino Corma (ITQ – CSIC / UPV, Spain)
Pedro Miguel Echenique (DIPC, Spain)
Kostya Novoselov (NGI - The University of Manchester, UK)

Keynote Speakers
Jouni Ahopelto (VTT, Finland)
Javier Aizpurua (CSIC-UPV/EHU, Spain)
Maya Bar-Sadan (Ben-Gurion university of the Negev, Israel)
Francesco Bonaccorso (IIT, Italy)
Paolo Bondavalli (Thales Research & Technology, France)
Mads Brandbydge (Technical University Denmark, Denmark)
Daniele Cangialosi (CFM-UPV/EHU-CSIC, Spain)
Remi Carminati (Langevin Institute - ESPCI, France)
Antonio Castro-Neto (NUS, Singapore)
Liraz Chai (The Hebrew University of Jerusalem, Israel)
Jean-Christophe Charlier (UCL, Belgium)
Karl S. Coleman (Durham University, UK)
Juan Carlos Cuevas Rodriguez (UAM, Spain)
Mihaela Delcea (University of Greifswald, Germany)
Jannick Duchet-Rumeau (IMP@INSA, INSA Lyon-GDR CNRS, France)
Alain Dufresne (Grenoble INP-Pagora, France)
Xinliang Feng (TU-Dresden, Germany)
Joaquín Fernández-Rossier (INL, Portugal)
Oleg Figovsky (Polymate Ltd., Israel)

Marta Fortea (University of Vienna, Austria)
Costas Galiotis (FORTH/ ICE-HT and University of Patras, Greece)
Francisco J. Garcia Vidal (UAM, Spain)
Jean-Jacques Greffet (Institut d'Optique Graduate School, France)
Elad Gross (The Hebrew University of Jerusalem, Israel)
Ariel Ismach (Tel Aviv University, Israel)
Alexander Kotlyar (Tel Aviv University, Israel)
Peter Koval (DIPC, Spain)
Yogendra Kumar Mishra (Kiel University, Germany)
Jose Maria Lagaron (IATA-CSIC, Spain)
Daniel Lanzillotti Kimura (C2N-CNRS, France)
Pascal Larregaray (CNRS / Université Bordeaux · ISM, France)
Max Lemme (AMO GmbH, Germany)
Luis Liz-Marzan (CIC Biomagune, Spain)
Liberato Manna (IIT, Italy)
Carmen Mijangos (CSIC/ICTP, Spain)
Rodolfo Miranda (IMDEA-Nanociencia, Spain)
Daniel Navarro-Urrios (ICN2, Spain)
Pablo Ordejón (ICN2, Spain)
Vincenzo Palermo (ISOF-CNR, Italy)
Alain Pénicaud (CNRS / Université Bordeaux-I, France)
Alessandro Pitanti (NEST, CNR-Nano, Italy)
Danny Porath (The Hebrew University of Jerusalem, Israel)
Victor Puntes (ICN2, Spain)
Stephan Roche (ICREA/ICN2, Spain)
Teófilo Rojo (CIC energigune, Spain)
Adi Salomon (Bar-Ilan University, Israel)
Roy Shenhar (The Hebrew University of Jerusalem, Israel)
Uri Sivan (Technion - Israel Institute of Technology, Israel)
Clivia Sotomayor Torres (ICREA/ICN2, Spain)
Soren Stobbe (Technical University of Denmark, Denmark)
Mauricio Terrones (The Pennsylvania State University, USA)
Ewold Verhagen (AMOLF, The Netherlands)
Robert Westervelt (Harvard University, USA)
Robert Young (The University of Manchester, UK)

Invited Speakers
Nassia Athanassiou (Istituto Italiano di Tecnologia, Italy)
Adolfo Benedito (AIMPLAS, Spain)
Peter Boggild (Technical University of Denmark, Denmark)
Mallika Bohm (Talga Technologies Ltd, UK)
Marc Chaigneau (HORIBA Scientific, France)
Ahmed Elmarakbi (University of Sunderland, UK)

Francisco José Fernández-Carretero (Tecnalia, Spain)
Aran García-Lekue (DIPC, Spain)
Julio Gomez (Avanzare, Spain)
Pedro Gomez-Romero (ICN2, Spain)
Stijn Goossens (ICFO, Spain)
Maria Jadraque (PONS IP, Spain)
Maria Jorda Beneyto (ITENE, Spain)
Priscila Kosaka (IMM-CNM-CSIC, Spain)
JingCheng Li (NanoGUNE, Spain)
Miguel Angel López Manchado (ICTP - CSIC, Spain)
David Mecerreyes (POLYMAT - UPV/EHU, Spain)
Cesar Merino Sanchez (Grupo Antolin Ingenieria, Spain)
Andrew J. Pollard (National Physical Laboratory, UK)
Albert Redo-Sanchez (das Nano S.L., Spain)
Anna Roig (ICMAB-CSIC, Spain)
Luis Sanz Tejedor (OEPM, Spain)
Felicien Schopfer (LNE, France)
Juan Jose Vilatela (IMDEA, Spain)
Helge Weman (NTNU & CrayoNano AS, Norway)
Rune Wendelbo (Abalonyx, Norway)
Anil O. Yalcin (Thermo Fisher Scientific, Netherlands)
Amaia Zurutuza (Graphenea, Spain)

Industrial Forum
Arantxa Ballesteros (ITENE, Spain)
Bojan Boskovic (Cambridge Nanomaterials Technology, UK)
Inmaculada Cabrera (CDTI, Spain)
Felix Casanova (NanoGune , Spain)
Iñigo Charola (Graphenea, Spain)
Antonio Correia (Phantoms Foundation, Spain)
Mª Pilar de Miguel (CDTI, Spain)
Mª Pilar de Miguel (CDTI, Spain)
Camila Delpivo (LEITAT, Spain)
Cristina Elizetxea (TECNALIA, Spain)
Carlos Fito (ITENE, Spain)
Sonia Florez (TECNALIA, Spain)
Alberto Garcia Luis (Tecnalia, Spain)
Mónica García-Mota (SIMUNE, Spain)
Nieves González (CDTI, Spain)
Albert Guerrero (IMB-CNM/CSIC, Spain)
Angel Hernan (SISTEPLANT, Spain)
Peter Koval (DIPC, Spain)
Sandrine Lebigre (R&D Programmes Manager (IPC), France)

Martin Lohe (TUD / cfaed, Germany)
Jesus Lopez de Ipiña (TECNALIA, Spain)
Javier Maira (CSIC, Spain)
Federico Marchesin (SIMUNE, Spain)
Cesar Merino Sanchez (Grupo Antolin Ingenieria, Spain)
Vincent Morin (RAITH GmbH, Germany)
José Mª Navas (INIA, Spain)
Frank Nouvertné (RAITH GmbH, Germany)
Ahmet Oguz Tezel (Graphene Batteries, Norway)
Mario Ordoñez (MTC, Maier Technology Center, Spain)
Simon Perraud (CEA, France)
Raquel Puelles (AVANZARE, Spain)
Isabel Rodriguez (GAIKER, Spain)
Blanca Suarez (TEMAS, Switzerland)
Ravi Sundaram (Oxford Instruments, UK)

Functional Polymers

March 19-21 2018
Centro de Física de Materiales CSIC-UPV/EHU, Donostia / San Sebastián
www.fz-juelich.de/jcns/FunctPolym2018

Organizing Committee
Juan Colmenero (CFM, CSIC-UPV/EHU)
Dieter Richter (Forschungszentrum Jülich, Germany)
Josexto Pomposo (CFM, CSIC-UPV/EHU)
Angel Moreno (CFM, CSIC-UPV/EHU)
Arantxa Arbe (CFM, CSIC-UPV/EHU)

The workshop focused on advanced polymer materials bringing together physicists and chemists who are interested in novel polymer nano-composites, polymers functionalized with supramolecular groups and functional soft nano-objects:
❖ Single chain nano-particles (SCNPs) display a molecular architecture containing multiple locally compact, but accessible, sites/cavities/zones so-called "local pockets" offering the possibility to anchor, either temporally or permanently, active species like e.g. catalysts or drugs.
❖ One-component nano-composites (OCNC) overcome the dispersion challenge and are expected to display structure related 'emergent' properties that make them unique within the general field of nano composites (NC).
❖ Polymers functionalized with reversible linkers (SUPRA) form offer superior properties compared to their non-associating counterparts. Supramolecular linkers introduce additional functionality such as self-healing, responsiveness, directed self-assembly or self-organization.

There were 14 invited talks (5 corresponding to SCNPs topic; 4 to OCNC and 5 to SUPRA). The corresponding invited speakers were from different countries: 6 from USA; 3 from Germany; 1 from Greece; 1 from the Netherlands; 1 from UK; 1 from Israel; and 1 from Spain. Apart from the invited speakers, there were 23 oral contributions and a Poster Session where 9 posters were presented. In the spirit of this type of 'hot topics workshops' we used to organize at DIPC, there were many discussions and interactions among the different participants and general aspects and concepts within the different topics were detected and highlighted.

Invited speakers
Alfredo Alexander-Katz (MIT, Boston, USA)
Mark Dadmun (University of Tennessee, Knoxville, USA)
Gabriel Lemcoff (Ben Gurion University, Beer-Sheva, Israel)
Jens-Uwe Sommer (Leibniz-Institute of Polymer Research, Dresden, Germany)
Michael R. Bockstaller (Carnegie Mellon University, Pittsburgh, USA)
Sanat K. Kumar (Columbia University, New York, USA)
Dieter Richter (Forschungszentrum Jülich GmbH, Jülich, Germany)
Dimitris Vlassopoulos (FORTH, Heraklion, Greece)
Mitchell Anthamatten (University of Rochester, Rochester, USA)
Margarita Kruteva (Forschungszentrum Jülich GmbH, Jülich, Germany)
Michael Rubinstein (University of North Carolina, Chapell Hill, USA)
Rint Shijbesma (Eindhoven University of Technology, Eindhoven, Netherlands)
Zuowei Wang (University of Reading, Reading, UK)
Angel Moreno (Centro de Física de Materiales (CSIC-UPV/EHU), San Sebastián, Spain)

International Spring School on High Performance Computing

April 23-27, 2018
Centro Ignacio María Barriola, UPV/EHU, Donostia / San Sebastián
http://grammars.grlmc.com/HighPer2018/

Organizing Committee
Materials Physics Center (CSIC-UPV/EHU), Donostia / San Sebastián
DIPC, Donostia / San Sebastián
Rovira i Virgili University, Tarragona

HighPer 2018 was a research training event with a global scope aiming at updating participants about the most recent advances in the critical and fast developing area of high performance computing, which covers a large spectrum of current exciting research and industrial innovation with an extraordinary potential for a huge impact on scientific discoveries, medicine, engineering, business models, and society itself. Renowned academics and industry pioneers lectured and shared their views with the audience.

Most subareas of high performance computing were displayed, from foundations, infrastructure and management to applications. Major challenges in the field wereidentified through 2 keynote lectures, 24 five-hour and fifteen-minute courses, and 1 round table, which tackled the most active and promising topics. Interaction will be a main component of the event. An open session gave participants the opportunity to present their own work in progress in 5 minutes. Moreover, there were two special sessions with industrial and recruitment profiles.

Invited Speakers
Tony Hey (Rutherford Appleton Laboratory, UK Science and Technology Facilities Council)
Srinivas Aluru (Georgia Institute of Technology)
David A. Bader (Georgia Institute of Technology)
Ümit V. Çatalyürek (Georgia Institute of Technology)
Alan Edelman (Massachusetts Institute of Technology)
Richard Fujimoto (Georgia Institute of Technology)
Timothy C. Germann (Los Alamos National Laboratory)
Lennart Johnsson (University of Houston)
Alfio Lazzaro (University of Zurich)
Andrew Lumsdaine (Pacific Northwest National Laboratory)
Madhav Marathe (Virginia Polytechnic Institute and State University)
Frank Mueller (North Carolina State University)
Adrian Sandu (Virginia Polytechnic Institute and State University
Vivek Sarkar (Georgia Institute of Technology)
Marc Snir (University of Illinois at Urbana-Champaign)
Josep Torrellas (University of Illinois at Urbana-Champaign)
Todd J. Treangen (University of Maryland, College Park)
Elena Vataga (University of Southampton)
Uzi Vishkin (University of Maryland, College Park)
David Walker (Cardiff University)

Euskal Esperientziak Zientzia Zabalkuntzan (EEZZ18)

June 14-15, 2018
Miramar Palace, Donostia-San Sebastián
http://eezz18.dipc.org

Organizing Committee
Amaia Arregi (DIPC)
Uxune Martinez (UPV/EHUko KZK)
Jon M. Matxain (UPV/EHU-DIPC)
Idoia Mugika (MFZ-CFM)

At EEZZ18 different initiatives that are undertaken to disseminate science in the Basque Country were presented. Thus, professionals working both at science communication and dissemination institutions and media, agents for informal STEM education, researchers, science lovers and cultural entrepreneurs, science teachers and students participated in the meeting.

The main goals follow:
❖ The complete the overall map of the multiple science dissemination initiatives in the Basque Country.
❖ To create a forum for the agents working in science diffusion.
❖ To create a network for collaboration between different science dissemination agents working in Basque.
❖ To reflect about how to become more effective.

Invited Speakers
Xabier Artaetxeberria (Ingeniaria)
Josu Ceberio (Zientziaren Giltzak Elkartea)
Larraitz Etxeberria (Eureka! Zientzia Museoa)
Luis Fernandez (Codesyntax)
Virginia Garcia (Aranzadi Zientzia Elkartea)
Carlos Garcia (Berritzegune)
Miren Karmele Gomez (Iruñeako Planetarioa)
Galder Gonzalez (Wikipedia Elkartea)
Maria Luz Guenaga (Deustuko Unibertsitatea)
Iñaki Gurrutxaga (EITB, Kosmos)
Arantxa Iraola (Berriako Kazetaria)
Aitziber Lasa (Elhuyar Fundazioa)
Jabi Luengo (Herrikide Ikastetxeko Irakaslea)
Zuriñe Maguregi (Gaztezuloko Zuzendaria)
Idoia Mugika (Materialen Fisikako Zentrua)
Itziar Otegui (CIC-Nanogune)
Juan Ignacio Perez (UPV/EHUko KZK)
Txelo Ruiz (UPV/EHU, e-makumeak)
Itziar Uribe (InnoBasque)
Itziar Zubia (UPV/EHU, Zientzia Astea)

Novel 2D materials explored via scanning probe microscopy & spectroscopy

June 25-29, 2018
Miramar Palace, Donostia / San Sebastián
http://2dspm.dipc.org/

Organizing Committee

Miguel M. Ugeda (DIPC-CFM)

Iván Brihuega (UAM-IFIMAC)

Scientific Committee

Mike Crommie (UC Berkeley – LBNL)

Miquel Salmerón (LBNL)

Nacho Pascual (CIC nanoGUNE)

Francisco Guinea (U. Manchester - IMDEA)

Technical Committee

Eva Cortés-del Río (UAM, Spain)

Diego Expósito (UAM, Spain)

Carmen Rubio (CIC nanoGUNE, Spain)

Javier Zaldivar (CIC nanoGUNE, Spain)

Since its abrupt emergence in 2004, 2D materials have concentrated the research efforts of a large portion of the scientific community. Those novel materials combine tantalizing fundamental properties with the most promising applications. In 2D materials, essentially everything takes place on the surface and, consequently, SPM techniques have produced some of the most exciting works in these unique materials. 2DSPM international conference brought together a good number of the leading researchers on the field. The aim was to provide a very stimulating environment facilitating the easy flow of knowledge and ideas between participants.

Invited Speakers

Michael Crommie (UCB & LBN, US)
Joseph Stroscio (NIST, US)
Eva Andrei (Rutgers, US)
Michael Fuhrer (Monash U., Australia)
Abhay Pasupathy (Columbia, US)
Harald Brune (EPFL, Switzerland)
Tim Wehling (U. Bremen, Germany)
Thomas Michely (U. Köln, Germany)
Markus Morgenstern (RWTH-Aachen, Germany)
Peter Wahl (U. St Andrews, Scotland)
Katharina Franke (FU. Berlin, Germany)
Rubén Pérez (UAM, Spain)
Jean –Y. Veuillen (I. Néel, France)
Jürg Osterwalder (UZH Physik, Switzerland)
Chih-Kang Shih (U. Texas, US)
Oleg Yazyev (EPFL, Switzerland)
Joaquín Fernández-Rossier ((INL Portugal)
Philip Hofmann (iNANO, Denmark)
Guy Le Lay (Marseille U., France)
Rodolfo Miranda (UAM, IMDEA, Spain)
José Ignacio Pascual (nanoGUNE, Spain)
Roland Wiesendanger (U. Hamburg, Germany)
Steven Louie (UCB, US)

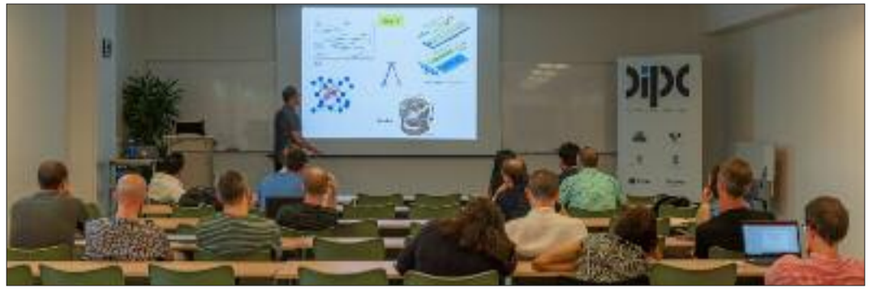
Single Atom Ba Tagging (SABAT)

July 9-10, 2018
DIPC, Donostia / San Sebastián
http://sabat2018.dipc.org/

Organizing Committee
JJ Gómez-Cadenas (DIPC)
D. Nygren (UTA)
Francesc Monrabal (UTA and DIPC)
Ben Jones (UTA)

The DIPC Workshop on "Single Atom Ba Tagging" (SABAT 2018) was held at the Donostia International Physics Center (DIPC), Donostia / San Sebastián, on July 9-10, 2018. The aim of the workshop wass to review the experimental techniques needed to achieved single-atom tagging in Xe-137 double beta decays produced in a gas xenon TPC. Currently, the most promising way to achieve Ba++ tagging is the use of Single Molecule Fluorescence Imaging. The notion, was proposed by Dave Nygren in 2017, and a first proof of concept has been carried out by the NEXT collaboration in 2018. Further progress requires a multi-disciplinary approach involving several fields. In the spirit of DIPC Workshops, SABAT provided a friendly atmosphere to foster discussions and collaborations between leading scientists working in the various fields involved.

Topics included:
- Applying Single Molecule Fluorescence Imaging to single-Ba++ ion tagging.
- Proof of principle of SMFI technique for Ba++ tagging.
- Developments of dyes for SMFI Ba++ tagging.
- SMFI Ba++ tagging in vacuum. Molecule layers and microscopy.
- SMFI Ba++ tagging in high pressure gas.
- Use of nano-technology to amplify signal.
- Development of Ba++ sources.
- Development of RF "carpets" for Ba++ collection.
- Implementation in HPXe chambers (e.g, NEXT detector).



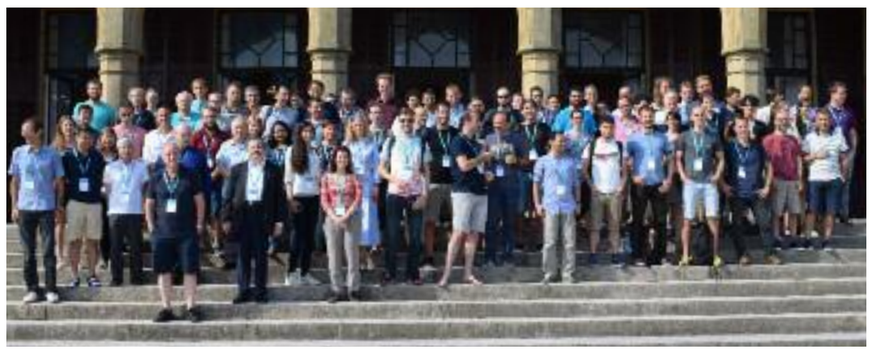
Invited Speakers
Barak Deyan (Weissman Institute)
Rubén Esteban (DIPC)
Álvaro Peralta (CLPU)
Fernando Cossio (UPV-EHU)
Celia Rogero (CFM)
Luca Salassa (DIPC)
Carlos Peña-Garay (LSC)
Dave Nygren (UTA)
Austin MacDonald (UTA)
Franck Foss (UTA)
Fernanda Psihas (UTA)
Edam Bainglass (UTA)
Ben Jones (UTA)

Quantum Designer Physics

July 16-19, 2018
Miramar Palace, Donostia / San Sebastián
http://qdp2018.dipc.org/

Organizing Committee
Daniel Loss (University of Basel)
Francisco Guinea (University of Manchester)
Andres Arnau (Materialen Fisika Zentroa CFM-UPV/EHU and DIPC)
Vitaly Golovach (Materialen Fisika Zentroa CFM-UPV/EHU, DIPC, and Ikerbasque Foundation)

The workshop Quantum Designer Physics will highlight recent advances in material systems purposefully designed for studying some of the most intriguing physical phenomena at the nanoscale. Very broadly these phenomena are related to spin, topology, and coherence, which enable the materials display quantum functionalities. Condensed Matter Physics is known for providing a rich variety of material systems in which different physics can be found and studied. With the recent development of quantum materials, it appears to be possible to devise the physics and implement a suitable material system for that physics on demand. This workshop brings together the leading experts working on quantum materials and aims at creating a stimulating atmosphere for discussing new physics on the marvelous sites of San Sebastian. We will discuss 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 will update 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 are also on our agenda. We hope the workshop will foster collaborations and inspire its attendants to tackle new problems with great ideas which make a difference for fundamental physics, lead to applications, and advance futuristic technologies.



Invited Speakers
Ramon Aguado (ICMM, CSIC, Madrid)
Yoichi Ando (University of Cologne)
Sebastian Bergeret (CFM-CSIC Donostia)
Miguel Angel Cazalilla (National Tsing Hua University, Taiwan)
Luca Chirolli (IMDEA Nanoscience)
Silvano De Franceschi (CEA Grenoble)
Fernando De Juan (University of Oxford)
Claudia Felser (Max Planck Institute for Chemical Physics of Solids, Dresden)
Duncan Haldane (Princeton University)
Pablo Jarillo-Herrero (Massachusetts Institute of Technology)
Georgios Katsaros (IST Austria)
Philip Kim (Harvard University)
Jelena Klinovaja (University of Basel)
Takis Kontos (Paris ENS)
Leo Kouwenhoven (Delft University of Technology and Microsoft Station Q Delft)
Charles Marcus (Niels Bohr Institute and University of Copenhagen)
Alberto Morpurgo (University of Geneva)
Mikhail Otrokov (Donostia International Physics Center)
Stuart Parkin (Max Planck Institute of Microstructure Physics and Martin Luther University of Halle-Wittenberg)
Jason Petta (Princeton University)
Christian Schönenberger (University of Basel)
Pascal Simon (Université Paris Sud)
Jairo Sinova (Johannes Gutenberg University Mainz)
Seigo Tarucha (The University of Tokyo and RIKEN Center for Emergent Matter Science)
Sergio Valenzuela (Catalan Institute of Nanoscience and Nanotechnology)
Felix von Oppen (Free University of Berlin)
Roland Wiesendanger (University of Hamburg)
Amir Yacoby (Harvard University)
Ali Yazdani (Princeton University)
Floris Zwanenburg (University of Twente)

New Generation in Strongly Correlated Electrons Systems (NGSCES 2018)

September 3-7, 2018
Miramar Palace, Donostia / San Sebastián
http://ngsces2018.dipc.org

Organizing Committee
Santiago Blanco-Canosa (CIC nanoGUNE and DIPC, Donostia / San Sebastian)
George Booth (King's College London)
Wojciech Brzezicki (International Research Centre MagTop, Warsaw)
Ion Errea (DIPC, Donostia / San Sebastian)
Matteo Minola (Max Planck Institute for Solid State Research, Stuttgart)
Laurenz Rettig (Fritz Haber Institute, Berlin)

The 9th international conference "New Generation in Strongly Correlated Electrons Systems" (NGSCES 2018), sponsored by the Donostia International Physics Center (DIPC), was held at the Miramar Palace in Donostia / San Sebastian, on September 3-7, 2018. The aim of the conference was to review the state of the art and new trends in the theoretical understanding and experimental investigation of strongly correlated electron systems. In the spirit of the previous successful NGSCES editions, we provided a friendly atmosphere to foster discussions and collaborations in particular between emergent and more experienced scientists in the field of correlated electron systems, by encouraging participation of researchers at an early stage of their career. For this purpose, the program of the conference also included many oral and poster presentations chosen among the contributed abstracts.

Topics included:
- Non-equilibrium Quantum Dynamics
- Topological Insulators and Spin-Orbit Coupled systems
- Strong Correlations on the Nanoscale
- Quantum Magnetism
- Unconventional Superconductivity
- Development of novel computational / experimental techniques in correlated condensed matter.

Invited Speakers
Dr. E. Benckiser (Max Planck Institute for Solid State Research, Stuttgart, Germany)
Dr. G. Carleo (ETH Zürich, Switzerland)
Dr. F. Cilento (Elettra Synchrotron, Trieste, Italy)
Dr. D. di Sante (Universität Würzburg, Germany)
Dr. G. Fugallo (Polytech, Nantes, France)
Prof. A. Frañó (UCSD, San Diego, USA)
Dr. T. Hyart (University of Leipzig, Germany)
Dr. J. Leblanc (Memorial University of Newfoundland, Canada)
Prof. C. Monney (University of Fribourg, Switzerland)
Dr. D. O'Regan (Trinity College, Ireland)
Dr. J. Schlappa (XFEL, Hamburg, Germany)
Dr. M. Sentef (Max Planck for Structural Dynamics, Hamburg)
Prof. W. Tabis (Uni. Vienna / Uni. Krakow, Austria/Poland)
Dr. J. Tomczak (TU Viena, Austria)
Dr. M.M. Ugeda (Materials Physics Center, San Sebastian, Spain)
Dr. M.G. Vergniory (Donostia International Physics Center, San Sebastian, Spain)
Prof. K. Wohlfeld (Warsaw University, Poland)

Spins on Surfaces (SoS II)

September 10-14, 2018
Miramar Palace, Donostia / San Sebastián
http://sos2.dipc.org

Organizing Committee
Deung-Jang Choi (CFM, CSIC-UPV/EHU and DIPC, Spain)
Andreas Heinrich (Center for Quantum Nanoscience, Korea)

The Scanning Tunneling Microscope is giving unprecedented insight into magnetic phenomena on the atomic scale. The objective of this meeting was to share the state-of-the-art among the actors in this field, as well as among interested students/researchers in related areas. Following the very successful SoS meeting of 2016 at the Miramar Palace, we hosted a second SoS workshop. The topic is timely and in expansion. We increased the original scope of the workshop to include the very exciting developments in quantum information thanks to the new ability of the scanning tunneling microscope (STM) to measure and control quantum spins. The workshop was devoted to the study of single magnetic moments on solid surfaces, their detection, manipulation, and encoding of quantum information. The single magnetic moments can be in atomic or molecular form, both systems having interesting properties to explore. Of great interest, the detection of spin resonance signal is becoming a landmark, and it is important to keep updated in this quickly developing field. The problems of correlations and the building in of information by manipulation and assembling quantum objects in a bottom up approach will also be a key component of the workshop. Finally, the introduction of superconducting substrate is giving a new twist to the field thanks to the complex behaviour of Cooper pairs in the context of magnetic local moments. This has led to the suggestion of creating Majorana fermions with tremendous implications on the field of quantum information. The Majorana fermions signal a topological phase of the superconducting substrate. Not only are they a new phase of matter but they have exotic transformation properties that permit to encode quantum computation. Due to their topological character, the new quantum operations are free of decoherence, becoming a new standard in quantum technologies.

Topics included:

- Single-atom magnetic inelastic spectroscopy.
- Single-molecule magnetic inelastic spectroscopy.
- Localized moments on different substrates: metals, insulators, superconductors, topological insulators.
- Spin dynamics on adsorbed atoms: T1 and T2 measurements and calculations.
- Electron spin resonance on a single atom.
- The Kondo effect.
- Entanglement in few-atom systems.
- Qubits on the atomic scale.

Invited Speakers
Andreas Heinrich (QNS-IBS, Korea)
Markus Ternes (University of Aachen, Germany)
Sander Otte (Delft University of Technology, Netherland) Sebastian Loth (University of Stuttgart, Germany)
Harald Brune (EPFL, Switzerland)
Pietro Gambardella (ETH, Switzerland)
Nicolas Lorente (CFM&DIPC, Spain)
Young Kuk (Seoul National University, Korea)
Jens Wiebe (University of Hamburg, Germany)
Joseph Stroscio (NIST, USA)
Alex Khajetoorians (Radboud University, Netherland) Katharina Franke (Free University, Germany)
Christian Ast (Max Planck Institute, Germany)
Joaquin Ferandez (University of Alicante, Spain) Deung-Jang Choi (CFM&DIPC, Spain)
Tim Wehling (Univeristy of Bremen, Germany)
Leo Gross (ETH, Switzerland)
Chris Lutz (IBM, USA)

Theoretical Methods in Molecular Spintronics

September 17-20, 2018
CFM, CSIC-UPV/EHU, Donostia-San Sebastián, Spain
http://tmspin.dipc.org/

Organizing Committee
Andrea Droghetti (Universidad del País Vasco, Donostia / San Sebastian)
Ivan Rungger (National Physical Laboratory, Teddington, UK)
Tim Wehling (University of Bremen, Bremen, Germany)

Magnetic molecules and atoms studied by scanning probe microscope experiments and molecular transistors represent ideal systems to address the very foundations of the quantum theory of magnetism. This workshop gathered both physicists and chemists to question what electronic structure theory to use for such systems. Hence, the most recent developments in first-principles methods were presented with a special focus on those that could describe correlation effects, excitations and complex structural details on equal footing.

Topics included:
❖ Magnetic properties of molecules in the gas phase, in particular spin state energetics and exchange coupling between several magnetic centers.
❖ Magnetic properties of atoms and molecule on surfaces, in particular the Kondo effect and surface-mediated exchange-coupling between adsorbed atoms,
❖ Finite-bias transport and magnetic excitations at the atomic scale,
❖ Entangled states and application to quantum computation in magnetic molecules and atoms.

In the spirit of DIPC and Psi-K, the workshop provided a friendly atmosphere to foster discussions and collaborations between physicists, materials scientists and quantum chemists. We planned to have mostly oral contributions by invited speakers. However, we encouraged the participation of postgraduate students and researchers at the early stage of their career, who submitted an abstract for a poster presentation. A few of these were selected to talk.

Invited Speakers
Jan Aarts (University of Leiden)
Marco Aprili (CNRS-Paris)
Norman Birge (Michigan State University)
Mark Blamire (University of Cambridge)
Silvano De Franceschi (CEA Grenoble)
Matthias Eschrig (Royal Holloway, London)
Mikael Fogelström (Chalmers)
Katharina Franke (Freie Universität Berlin)
Francesco Giazotto (CNR-Pisa)
Sophie Gueron (LPS-Orsay)
Ewelina Hankiewicz (Würzburg Univ.)
Tero Heikkilä (University of Jyväskylä)
Leo Kouwenhoven (Delft)
Yoshi Maeno (University of Kyoto)
Dirk Manske (MPI-Stuttgart)
Julia Meyer (CEA Grenoble)
Oded Millo (University of Jerusalem)
Jagadeesh Moodera (MIT)
Stuart Parkin (MPI, Halle)
Dimitri Roditchev (INSP Paris)
Ilya Tokatly (University of Basque Country)
Javier Villegas (CNRS-Thales)
Felix von Oppen (FU Berlin)

On-Surface Synthesis International Workshop (OSS-18)

September 24-28, 2018
Sant Feliu de Guíxols, Girona, Spain
http://oss18.dipc.org

Scientific Committee
Roman Fasel (EMPA, Switzerland)
Wei Xu (Tongji University, China)
Florian Klappenberger (Technische Universität München, Germany)
Michael Crommie (University of California at Berkeley, USA)

Organizing Committee
André Gourdon (CEMES-CNRS, France)
Dimas G. de Oteyza (Donostia International Physics Center, Spain)
Nian Lin (The Hong Kong University of Science and Technology, Hong Kong)
Andrej Jankarik (CEMES-CNRS, France)

On-surface synthesis unites the easy tunability of molecular materials and the promises of self-assembly as a revolutionary production method, with the sturdiness of covalently bonded structures. This most attractive combination is drawing the interest of a rapidly increasing number of researchers. Important efforts are being devoted to augment the still scarcely equipped on-surface synthesis toolbox, to improve our understanding of the chemical reaction mechanisms, as well as to the synthesis and characterization of new molecular architectures of potential use in diverse applications.

Because this approach bridges across the fields of chemistry, physics and materials science, the aim of this third edition of the "On-Surface Synthesis" international workshop was to bring together researchers working in this field from different perspectives. Doing so we provided a diverse and stimulating environment to present and discuss the present, past and future of this novel and promising synthetic route.

Invited Speakers
Roman Fasel, EMPA, Switzerland
Wei Xu, Tongji University, China
Florian Klappenberger, Technische Universität München, Germany
Michael Crommie, University of California at Berkeley, USA
Markus Lackinger, Technische Universität München, Germany
Diego Peña, Universidad de Santiago de Compostela, Spain
Francesca Moresco, Technische Universität Dresden, Germany
Michael Gottfried, Philipps-Universität Marburg, Germany
José Ignacio Pascual, CIC NanoGUNE, Spain
Jonas Björk, Linköping University, Sweden
Hironobu Hayashi, Nara Institute of Science and Technology, Japan
Sabine Maier, University Erlangen-Nürnberg, Germany
Leo Gross, IBM Zürich, Switzerland
Harald Fuchs, University of Münster, Germany

XIII International Ontology Congress

October 2-6, 2018
Chillida-Leku Museum, Donostia / San Sebastián
October 9, 2018
Confucius Institute, Barcelona
http://www.ontologia.info/es/index.php/last-edition

Organizing Committee
A. Aspect (Paris)
P. Aubenque (Paris)
F.J. Ayala (California)
J. Bouveresse (Paris)
E. Chillida (San Sebastián)
A. Grünbaum (Pittsburgh)
W. Lamb (Arizona)
T. Marco (Madrid)
U. Moulines (München)
I.Prigogine (Bruxelles)
H. Putnam (Boston)
C. Rovelli (Marseille)

Coordinator
V. Gómez Pin (Barcelona)

In 1964 Robert Brout and François Englert published an article in Physical Review Letters that delved into hypotheses already advanced by themselves. In this article they defended that a singular particle should be given in the category of the so-called bosons. A few months later, the Scottish scientist Peter Higgs advanced an analogous hypothesis. In 2012, the Brout-Englert hypothesis was verified. Unfortunately, too late for Robert Brout to enjoy this great moment of satisfaction... he had passed away in 2011. Great physicists, sometimes Brout's students, follow his scientific path. Philosophers, who are nourished by the results of the scientist's effort to make the nature intelligible, owe him, undoubtedly, tribute.

Since the first conference took place back in 1993, the aim of the International Ontology Congress, of which most of the conferences have been held under the auspices of UNESCO, has been to breathe new life into the great topics of Greek philosophy, examining them from a contemporary perspective, namely, using the tools provided by contemporary science. These problems keep being brought up constantly, either because of the emergence of new scientific data or because of the irruption of new philosophic perspectives.

It is obvious that the philosophical and ontological reflection about nature, what was in other times known as natural philosophy, cannot take place without the support of the "natural science of our times", in Heisenberg`s words. It is well known that in the first twenty-five years of the XX century, experimental facts showed that the classical picture of nature was not completely justified in the realm of the microscopic. This was not the consequence of a philosophical whim, but it was imposed on the scientific community by the progressive accumulation of facts impossible to accommodate inside the previous picture of nature.

The main ontological implications of the new discipline were shown at the 1927 Solvay conference. A.S. Eddington asserted later that, if it was confirmed, the collapse of Absolute Causality announced in Solvay by Heisenberg, Born and others would make of this meeting one of the crux moments of the scientific and philosophical thought. But, as the Royal Majesty in the verses of Shakespeare, Causality never dies alone: it sweeps along a whole set of entangled principles that, from Greek physikoi to Einstein, had been considered the very grounds of our representation of nature. From then (and in spite of new theoretical data and crucial experiments) we can say that many of the questions discussed in the Solvay conference remain open and nourish in our days a fascinating debate. We discussed these implications as well as created new avenues for discussion at the first main section we proposed for the XIII International Ontology Congress to be held in Donostia / San Sebastián, from the 2nd to the 6th of October 2018: Since "Solvay 1927": Nature and Quantum Physics (state of the art).

But it has not been the first time that philosophical problems rise in the history of Physics. In fact, the first West physicists, the thinkers of the marina cities of Ionia and their successors, were already confronted to deep questionings, which leaded to the advent of meta-physics, understood as the fate of Physics itself. This is why in 1948, Nobel Prize winner Erwin Schrödinger interrupted a course at Trinity College in Dublin arguing that, before continuing to work on physics, it was necessary for him to know the meaning of the word Physis. As he greatly admired the Greek intuition of scientific view, Schrödinger seemed to think that returning to the roots was the best way of staying faithful to the spirit of science. Then, let`s turn our attention to those roots, asking nevertheless if others civilizations were already developing an embryonic conception of nowadays physics. The International Ontology Congress maintains deep reliance on the roots, the foundations of current science and this confidence has been the inspiration for our second main section also to be held in Donostia / San Sebastián, from the 2nd to the 6th of October 2018: Back to Ionia: the conception of Physis that makes Physics possible.

Invited Speakers
François Englert (2013 Nobel Prize of Physics. Université Libre de Bruxelles)
Gerardus 't Hooft (1999 Nobel Prize of Physics. Utrecht University)
Tomás Calvo (Universidad Complutense de Madrid)
Francesc Casadesús (Universitat de les Illes Balears)
Elena Castellani (University of Florence)
Alberto Cordero (CUNY)
Joseph Dauben (CUNY)
Elie During (Université de Nanterre)
Pedro M. Echenique (Donostia International Physics Center)
Dimitri El Murr (ENS)
Jean-Marie Frère (Université Libre de Bruxelles)
J.J. Gómez Cadenas (Donostia International Physics Center)
Richard Healey (University of Arizona)
Carl Hoefer (Universitat de Barcelona)
Simon Kochen (Princeton University)
Michela Massimi (The University of Edinburgh)
Tim Maudlin (New York University)
Gérard Naddaf (York University)
Carlo Rovelli (Aix-Marseille Université)
Pilar Ruiz-Lapuente (Universitat de Barcelona)
Juha Saatsi (University of Leeds)
Ruediger Schack (Royal Holloway, University of London)
Gerhard Seel (University of Bern)
Demetra Sfendoni-Mentzou (Aristotle University of Thessaloniki)
Jesús Ugalde (Jakiunde, Academia de las Ciencias, de las Artes y de las Letras del País Vasco)
Peter Vickers (Durham University)
David Wallace (University of Southern California)
Francis Wolff (École Normale Supérieure)

Spanish Conference on Nanophotonics (CEN2018)

October 3-5, 2018
Carlos Santamaría Center (UPV/EHU), Donostia / San Sebastián
http://cen2018.dipc.org

Organizing Committee
Javier Aizpurua (CFM-UHV-CSIC)
Luis Liz-Marzán (Biomagune)
Rubén Esteban (DIPC)
Gabriel Molina-Terriza (CFM-UHV-CSIC)
Rainer Hillenbrand (CIC nanoGUNE)
Aitzol García-Etxarri (DIPC)
Juan José Sáenz (DIPC)

Scientific Committee
Gonçal Badenes (ICFO)
Francisco Meseguer (UPV-CSIC)
Salvador Balle (UIB)
Josep Pallarés (URV)
Enrique Calleja (UPM)
Jose Sánchez-Dehesa (UPV)
Francesc Díaz (URV)
José A. Sánchez Gil (IEM-CSIC)
Francisco J. García-Vidal (UAM)
Rosalia Serna (IO-CSIC)
Javier Marti (CTN-UPV)
Jan Siegel (IO-CSIC)
Juan Martínez-Pastor (ICMUV)
Clivia Sotomayor (ICN-CIN2)
Luís Viña (UAM)

The Conference aspired to address a wide range of topics related to nanophotonics, metamaterials and sub-wavelength optics. Topics included all aspects of research, ranging from fundamental science to fabrication and applications. Special sessions were devoted to emerging fields of research such as Quantum Nano-optics, spin-orbit coupling of light and topological photonics to mention a few.

CEN2018 took place in Donostia / San Sebastián following the spirit initiated by the first five editions of the Spanish Nanophotonics Conference held respectively in Tarragona (2008), Segovia (2010), Carmona-Sevilla (2012), Santander (2014) and Valencia (2016). The Conference aims to gather all the groups carrying out research in Nanophotonics in Spain (as well as somewhere else with interest in the research in Nanophotonics performed here). It intention is to spread the research results achieved by all the different Spanish groups and to promote the establishment or reinforcement of contacts between them, as a means to help the community to become more visible and dynamic.

The Conference was organized in thematic sessions composed of plenary, keynote and invited talks as well as contributed scientific communications (oral and poster). For a wider diffusion, contributions were in English.

Invited Speakers
Sir Michael V. Berry (University of Bristol, UK)
Nicholas Kotov (University of Michigan, USA)
Jeremy Baumberg (NanoPhotonics Centre, Cambridge, UK)
Maria García-Parajo (ICFO, Barcelona, Spain)
Javier García de Abajo (ICFO, Barcelona, Spain)
Francisco J. García Vidal (IFIMAC, Madrid, Spain)
María Losurdo (CNR-NANOTEC, Bari, Italy)
Isabel Pastoriza-Santos (Universidad de Vigo, Spain)
Mário Silveirinha (Universidade de Lisboa, Portugal)
Paloma Arroyo Huidrobro (Imperial College, London, UK)
Jorge Bravo Abad (IFIMAC, Madrid, Spain)
Andrés Castellanos (ICMM-CSIC, Madrid, Spain)
Elena del Valle (Universidad Autónoma de Madrid, Madrid, Spain)
Ivan Fernandez-Corbaton (Karlsruhe Institute of Technology, Germany)
Iñigo Liberal (Universidad Pública de Navarra, Spain)
Nerea Zabala (UPV-EHU, Bilbao, Spain)
Ramon Paniagua-Dominguez (A*STAR, Singapore)
Esther Alarcon Lladó (AMOLF, Netherlands)

HOPDSS2018

October 17-20, 2018
Miramar Palace, Donostia / San Sebastián
http://www.ehu.eus/ehusfera/hopdss2018/

Organizing Committee
Massimiliano Badino (University of Verona)
Arianna Borrelli (Technische Universität Berlin)
Edward A. Davis (University of Cambridge)
Christian Forstner (University of Frankfurt)
Greg Good (American Institute of Physcis)
Karl Grandin (Royal Swedish Academy of Sciences)
Gisela Mateos (Universidad Nacional Autónoma de México)
Jaume Navarro (Ikerbasque and University of the Basque Country)
José Manuel Sánchez-Ron (Universidad Autónoma de Madrid)
Peter M. Schuster (Echophysics, Pöllau, Austria)
Maria Rentetzi (National Technical University of Athens)
Xavier Roqué (Universitat Autònoma de Barcelona)
Iñaki San Pedro (University of the Basque Country)
George Vlachakis (Hellenic Open University and National Hellenic Research Foundation)
Denis Weaire (Trinity College, Dublin)

2018 marks the 50th anniversary of the creation of the European Physical Society (EPS). In this context, and following the success of two previous meetings in Cambridge (United Kingdom) and Pöllau (Austria), we are happy to announce the Third International Conference on the History of Physics, under the auspices of the EPS, which will take place in Donostia/San Sebastian (Spain) in October 17-21, 2018. The main goal of the conference is to provide a forum where historians of physics and physicists meet to reflect on the importance of the history of science for the development of contemporary physics, not only in its conceptual evolution but also at the institutional, organizational and educational levels; as well as to promote the contribution of practicing physicists to the highly professionalised discipline of the history of physics. On this occasion, this exchange will be enhanced by the joint celebration of the conference of early-career historians of physics, a bi-annual event sponsored by the History Center of the American Institute of Physics.

Invited Speakers
Patricia Fara (University of Cambridge)
James Bennett
Roberto Lalli (Max Planck Institute for the History of Science, Berlin)
Pablo Ruiz de Olano (Max Planck Institut für Wissenschaftsgeschichte)
Rudolf Meer (University of Graz)
Matthias Heymann (Aahrus Universitet)
Massimiliano Badino (University of Verona)
Raffaele Pisano (Université de Lille)
Erdmann Görg (Ruhr-Universität Bochum)

Ricardo Karam (Københavns Universitet)
Arianna Borrelli (Technische Universität Berlin)
Jan Lacki (Université de Genève)
Daniela Monaldi (York University)
Marij van Strien (Bergische Universität Wuppertal)
Helge Kragh (Københavns Universitet)
Marià Baig, Gonzalo Gimeno(Universitat Autònoma de Barcelona)
Enric Pérez (Universitat Autònoma de Barcelona)
Mercedes Xipell (Universitat Autònoma de Barcelona)
George Vlahakis (Hellen Open University and Inistitute for Historical Research)
Geert Vanpaemel (Katholieke Universiteit Leuven)
Santiago Sierra (Basque Association for Oriental Studies)
Carlos Hugo Sierra (Basque Association for Oriental Studies)
Thiago Hartz (Universidade Federal do Rio de Janeiro)
Reinaldo de Melo E Souza (Universidade Federal Fluminense)
Edward Davis (University of Cambridge)
Christopher Sinclair (Caterham School)
Bruno Nobre (Pontifical Catholic University of Rio de Janeiro)
Antonio Augusto Passos Videira (Pontifical Catholic University of Rio de Janeiro)
Marcos Paulo Da Cunha Martinho (Pontifical Catholic University of Rio de Janeiro)
Cormac O'Raifeartaigh (Waterford Institute of Technology)
Denis Weaire (Trinity College, Dublin)
James Lunney (Trinity College, Dublin)
Sian Stott (Univeristy of St Andrews)
Isobel Falconer (Univeristy of St Andrews)
Charles Baily (Univeristy of St Andrews)
Paul Cruickshank (Univeristy of St Andrews)
Andrew Whitaker (Queens University, Belfast)
Richard Staley (University of Cambridge)
Joanna Behrman (Johns Hopkins University)
Joseph D. Martin (University of Cambridge)
Xavier Roqué (Universitat Autònoma de Barcelona)
Katemari Rosa (Universidade Federal da Bahia)
Thomas Kaiserfeld (Lund University)
Climério Silva Neto (Universidade Federal do Oeste da Bahia)
Falk Müller (Goethe Universität)
Arne Schirrmacher (Humboldt Universität)
Nasser Zakariya (University of California, Berkeley)
Karl Grandin (Royal Swedish Academy of Sciences)
Juraj Sebesta (Univerzita Komenského)
Ganka Kamisheva (Bulgarian Academy of Sciences)
Pangratios Papacosta (Columbia College Chicago)
Juan Navarro-Loidi (Euskal Herriko Unibersitatea)
John Reid (University of Aberdeen)
Isabel Malaquias (Universidade de Aveiro)

Transborder QuantumChemPhys Lab Workshop

November 5-6, 2018
Bayonne, France
http://cen2018.dipc.org

Organizing Committee
Pascal Larregaray (Université de Bordeaux)
Ricardo Díez Muiño (Centro de Física de Materiales CSIC-UPV/EHU, DIPC)

Theoretical Chemistry and Physics at the Quantum Scale (QuantumChemPhys) is a Transborder Joint Laboratory (LTC - Laboratoire Transfrontelier Conjoint, http://www.quantumchemphys.org) created by Université de Bordeaux (UBx), Universidad del País Vasco / Euskal Herriko Unibertsitatea (UPV/EHU), and Donostia International Physics Center (DIPC). The purpose of the QuantumChemPhys lab is to strengthen the scientific collaboration among researchers from Euskadi and Aquitaine through the creation of a transnational institution focusing on the theoretical aspects of chemistry and physics at the quantum scale, i.e. the quantitative description of the motion of electrons and nuclei (and their coupling) in solids, at gas-solid interfaces, as well as in the interaction with light. Such a challenge requires the developments of theoretical methods and numerical simulations within the framework of quantum/classical/semiclassical mechanics.

In this context, the QuantumChemPhys Lab organized a workshop in which recent activity on the topics of interest to the Lab will be discussed. Approximately 35 scientists from the three institutions forming the QuantumChemPhys lab gathered in Bayonne. All PhD students that are developing their research project under the joint supervision of scientists in Donostia and Bordeaux had the opportunity to present their work in the workshop. The contribution of other junior researchers was icluded as well. Possibilities of further collaboration among the institutions forming the Transborder Lab were explored. This workshop contributes to keep the cohesiveness of the QuantumChemPhys lab, as well as building and developing new lines of research.

Invited Speakers
Quentin Schaerverbeke
Julie Baumard
Bogusz Bujnowski
Olatz Uranga
Alejandro Peña Torres
Alberto Rodríguez-Fernández
Claire Tonnelé
María Eugenia Sandoval-Salinas
Masoud Mansouri
Remi Avriller
Daniel Sánchez-Portal
César Ibargüen-Becerra
Elisa Jimenez-Izal
Sebastian P. Sitkiewicz
Carlos García Fernández
Alejandro Rivero Santamaria
Arnaud Desmedt
Andrés Arnau
Verónica Postils
Mireia Via-Nadal
Ion Mitxelena
Irene Casademont-Reig
Abel Carreras
Laurent Bonnet

From Bioinorganic Chemistry to Catalysis

23 November 2018
Faculty of Chemistry, UPV/EHU (Donostia)

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)
E. Tomás G. de Mendivil (UPV/EHU, 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 Prof. Patrick Gamez (ICREA Professor at the University of Barcelona).

Invited Speakers
Patrick Gamez (University of Barcelona, ICREA)
David de Sancho (UPV/EHU - DIPC)
Silvia Vera (UPV/EHU)
Enrique Gómez Bengoa (UPV/EHU)
Oihane Sanz (UPV/EHU)
David Rodriguez-Larrea (BIOFISIKA)
Oier Etxebeste (UPV/EHU)
Eder Tomas Gonzalez de Mendivil (UPV/EHU)

Software Carpentry

December 5-19, 2018
CFM and DIPC, Donostia / San Sebastián
http://cfm.ehu.eus/sc

Organizing Committee
Iñigo Aldazabal Mensa (CFM)

Software Carpentry aims to help researchers get their work done in less time and with less pain by teaching them basic research computing skills. This hands-on workshop covered basic concepts and tools, including program design, version control, data management, and task automation. Participants were encouraged to help one another and to apply what they learned to their own research problems.

The workshop was aimed to all CFM and DIPC research staff, as well as technicians, and was by no means only of interest to the theoretical people. People from other communities are welcome to attend, subject to seat availability.

Topics included:
❖ Introduction to shell scripting (Diego Lasa, DIPC)
❖ Popular software version control system 'git' (Inigo Aldazabal, CFM)
❖ Introduction to the Python programming language (David de Sancho and Sofia Sanz, DIPC) and
❖ Walkthrough over a typical (physics) data analysis workflow using some of its scientific and numerical libraries (Inigo Aldazabal, CFM)

Invited Speakers
Andrés Diaz-Gil (Institute for Theoretical Physics – CSIC-UAM, Madrid)
David de Sancho (DIPC)
Anita C. Schürch (University Medical Center Utrecht, Netherlands)

Higher Education

DIPC School

Topological Matter School 2018 180

DIPC Courses

Topology in Physics 181

Course on Neurophysics: From molecular channels to neural networks 181

Dynamical Mean-Field Theory 182

Theses 183

Master's Degree Program

UPV/EHU Research Master's in Nanoscience 184

DIPC School

Topological Matter School 2018

August 27-31, 2018
Miramar Palace, Donostia / San Sebastián
http://tms18.dipc.org/

Topology and lattice symmetries play a key role in determining matter states and their associated internal order. These so-called topological states of matters are of fundamental interest, since they entail exotic electronic behaviors. The study and prediction of materials with novel topological properties has become a vibrant field of research over the past few years. The main goal of the Topological Matter School 2018 was to cover basic and advanced aspects of the field. Over one week, the school provided extended lectures by leading experts on key aspects of topological matter:

❖ Graduate level presentations introducing the basic concepts of the field, including an introductory session on group theory and topological classification of matter.
❖ Several focus sessions on different topological phases (Weyls semi-metals, Majoranas fermions and topological superconductivity, non-symmorphic topological insulators, etc).
❖ A practical session on numerical exaclty solvable interacting model in one-dimensions.
❖ A review session on the major experimental achievements in the field.

While the school was primarily aimed at instructing master and graduate students and young postdoctoral researchers, more senior scientists who wanted to acquaint themselves with the subject of the school were-also welcome.

Invited Speakers
Alexander Altland (University of Cologne)
Haim Beidenkopf (Weizman Institute — Rehovot)
Andrei Bernevig (Princeton University)
Erwann Bocquillon (École Normale Supérieure — Paris)
Claudia Felser (Max Planck Institute — Dresden)
Joel Moore (University of California — Berkeley)
Titus Neupert (University of Zurich)
Stuart Parkin (Max Planck Institute — Halle)
Frank Pollmann (Technical university of Munich)
Leslie Schoop (Princeton University)
Andreas Schnyder (Max Planck Institute — Stuttgart)
Matteo Rizzi (Johannes Gutenberg University of Mainz)

DIPC Course

Topology in Physics

February 2018
DIPC, Donostia / San Sebastián

Dr. Nicolás Lorente
Centro de Física de Materiales, CSIC-EHU, and DIPC (Donostia-San Sebastián)

Topology is becoming a common place in today's physics research. It is however foreign and difficult to grasp to many of us. I will give an introductory presentation to this topic in 4 lectures of one hour and a half. The courses were detailed but with minimum mathematical requirements (all needed concepts were introduced). The main objective of the course was to give a handle on terminology and concepts that are regularly used. The syllabus for the course was:
❖ The adiabatic theorem and the Berry phase. Continuous deformation and topological invariants.
❖ The SSH model. Edge states and the bulk-boundary correspondance.
❖ Topological insulators.
❖ Topological superconductors. The "periodic table" of topological insulators and superconductors.

DIPC Course

Course on Neurophysics: From molecular channels to neural networks

March 2018
DIPC, Donostia / San Sebastián

Prof. Rafael Yuste,
Columbia University, NY (USA)

The course introduced modern neuroscience with especial emphasis on its connection to physics, both experimentally and theoretically. As a textbook, Prof. Yuste recommended:
Peter Sterling and Simon Laughlin, "Principles of Neural Design", The MIT Press, Cambridge Massachussetts (2015). This book is available at the DIPC library.

There were five lectures of one hour and a half each and can be found at the moodle of the course.
The topics were:
❖ Neuronal biophysics
❖ Neural anatomy and development
❖ Methods
❖ Neural networks
❖ Neural behavior and open questions

DIPC Course

Dynamical Mean-Field Theory

November 2018
DIPC, Donostia / San Sebastián

Dr. David Jacob
Ikerbasque Fellow (Donostia-San Sebastián)

With almost 30 years of existence, Dynamical Mean-Field theory (DMFT) is becoming a standard to go beyond Density Functional Theory in the systems where mean-field theory fails. Typical systems involve correlated centers that need some strongly-correlation treatment. DMFT uses a mapping into the Anderson impurity model, solving a Kondo problem and then modifies the mean-field solution of the non-correlated part by suitable self-energies that take into account the correlation.

Dr. David Jacob is an expert in the Kondo problem and in DMFT. He teaches the strongly-correlated problem in electronic structure calculations, DMFT and the limitations of DMFT.

The course consisted of four lectures of 90 minutes each, held in the DIPC seminar room:
❖ Motivation: Understanding the Mott Metal-Insulator transition;
The Hubbard model: Mean-Field solution; Gutzwiller Method.
❖ Dynamical Mean-Field Theory: the limit of infinite dimensions; DMFT in finite dimensions.
❖ Impurity solvers: NCA/OCA; Overview over other solvers.
❖ Failure of DMFT in low dimensions; Extensions of DMFT: Cluster DMFT;
Dynamical Cluster Approximation.

Theses

Chain dynamics in crosslinked filled and unfilled polymer blends of different miscibility.
Lucia Ortega Alvarez
16/03/2018
Supervisors: Silvina Cerveny and Gustavo Ariel Schwartz

Electronic and transport properties of 2D Dirac materials: graphene and topological insulators.
Bernhard Kretz
20/07/2018
Supervisor: Arantzazu García Lekue

Reduced density matrices: development and applications.
Mauricio Rodriguez Mayorga
24/07/2018
Supervisors: Eduard Matito and Miquel Sol

Theoretical study of the linear and nonlinear optical response of plasmonic tunneling gaps.
Garikoitz Aguirregabiria Achutegui
07/09/2018
Supervisors: Javier Aizpurua and Rubén Esteban

Theoretical studies on molecular adsorption and the effect of strain on core-level spectroscopy in different metal surfaces.
Anton Xosé Brión Ríos
15/10/ 2018
Supervisors: Pepa Cabrera and Daniel Sánchez Portal

Bioorthogonal photocatalytic activation of metal-based agents.
Silvia Alonso De Castro
26/10/2018
Supervisor: Luca Salassa

Electronic bands of nanoporous networks and one-dimensional covalent polymers assembled on metal surfaces.
Ignacio Piquero Zulaica
30/11/2018
Supervisors: Jorge Lobo-Checa and J. Enrique Ortega

Theory of plasmon-enhanced spectroscopy of molecular excitations: infrared absorption, fluorescence, and Raman scattering.
Tomas Neuman
14/012/2018
Supervisor: Javier Aizpurua

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 127 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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