DIPC 2015

Donostia International Physics Center

ON THE COVER **OCEAN OF SCATTERED SKIES**

Optical microscopy image of uniaxially aligned domains of terthiophene under crossed polarizers. The alignment results from a thermal gradient annealing process.

2015

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Science as a part of Culture

In the year 2000, not so long ago, the only building hosting research in physics and chemistry in the Ibaeta Campus of University of the Basque Country (UPV/EHU) was the UPV/EHU Chemistry Faculty. Animated by a group of young, brilliant, and enthusiastic scientists, which were starting from scratch, the Faculty soon became one of the best scientific spots of UPV/EHU. The explosion of scientific activity and, in particular, the potential foreseen for developing competitive research lines and projects in physics asked for a necessary growth of resources.

It is in this context that two centers were designed and created within a thoughtful strategy: the Centro de Física de Materiales (CFM), a joint center between UPV/EHU and Consejo Superior de Investigaciones Científicas (CSIC), and Donostia International Physics Center (DIPC). Together with Unidad de Biofísica (UPV/EHU-CSIC, in Leioa), they were the very first research centers launched in the Basque Country and paved the way for later institutional initiatives. The strategy was set up with a twofold goal: first, to attract and retain scientists that could develop world-class research, offering them the necessary stability to launch their scientific careers; second, to create an international and dynamical environment in which the interaction with top scientists from foreign institutions could be customary. The development of this plan would also catalyze the scientific activity in its close environment, putting Ibaeta Campus on the map of physics. Public institutions as well as some private companies rapidly adhere to the visionary scheme in an uncommon joint effort that showed the strategic weight of the proposal.

Not even the most optimistic predictions anticipated the success of the plot. This report on DIPC's activity in 2015 is living proof of that. Sixteen years after its opening, DIPC researchers have published more than 2,750 scientific articles which have received more than 70,000 citations; 10,700 of them in the year 2015. More than 100 workshops and 750 seminars have been organized and 2,500 researchers have visited DIPC to extend the frontiers of science. The numbers are indeed impressive but they do not tell the whole story. Actually, they do not tell even a bit of the story. The real success of DIPC has been to become a singular and flexible institution, a pole of attraction for scientists from all over the world that find in its facilities the creative and intellectually stimulating environment required to perform research at its highest level.

Ricardo Díez Muiño
Director

Back in 2000, when DIPC was opened, one of the most repeated statements, front-paged in many media, was the wish to transform Donostia/San Sebastián into a city of science, a place known not only for its beautiful landscape and welcoming gastronomy but also for its scientific activity. In 2016 we can say this dream is becoming a reality and at DIPC we are proud to have contributed to accomplishing this.

Donostia/San Sebastián, a city of science, but also science in the city.

This has been a motto for DIPC for many years. Science is not only for scientists. Science has to be owned and enjoyed by society as a whole. Science education is necessary to better understand and evaluate the advantages and risks of scientific and technological progress. For this reason, DIPC always looks for opportunities to bring science to the citizens. DIPC programs, such as *Kutxa Lectures*, *OnZientzia*, *top@DIPC*, and the *Passion for Knowledge* Festivals, among others, are developed to share the excitement of science with different social groups, especially with the youngest.

Pedro Miguel Echenique
President

Science is the most effective way to acquire new knowledge about the surrounding world and constantly reshapes our intellectual perspective. It is therefore an integral part of human culture. DIPC's activities in the city of Donostia/San Sebastián for 2016 are thus particularly relevant this year in which Donostia/San Sebastián has been designated European Capital of Culture. The 2016 Passion for Knowledge Festival, for instance, will be integrated into the official program of the initiative. The achievements of the scientists that develop their work in the different universities and research centers of Donostia/San Sebastián are splendid grounds to proudly display the title of European Capital of Culture. ■

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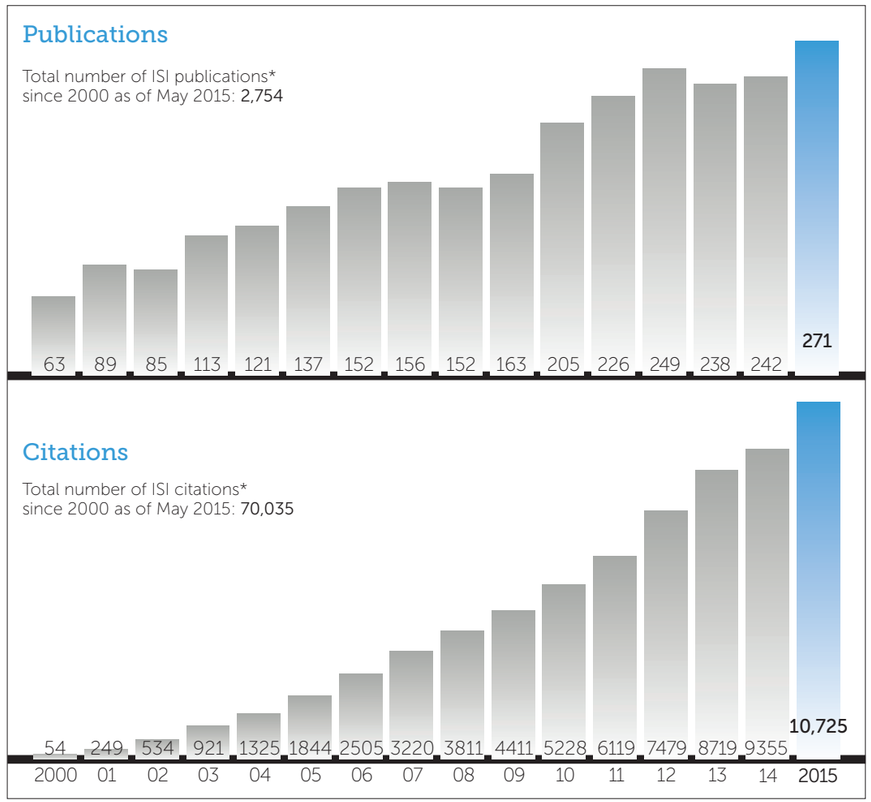
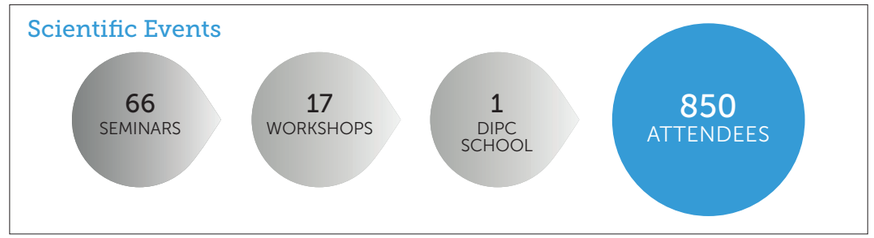
Research Activity at a Glance

DIPC's scientific production and international impact continually increases. The center has published a total number of 2,754 ISI publications. In just sixteen years since its initiation DIPC has more than quadrupled its number of publications and has received more than 70,035 citations.



*Source Web of Science Core Collection - DIPC's ResearcherID C-3171-2014 (06/05/2016)



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 which focus on learning particular skills.

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

In addition to PhD students and postdoctoral researchers, who come from other institutions to complete their training and expertise, the core of the DIPC community is made up of local scientists. Some of them are spread over other centers in different faculties of the University of the Basque Country and the Materials Physics Center and are distinguished such as the DIPC associates. The local scientists act as hosts for the large number of international visiting researchers and retain the scientific-technical knowledge in the local environment developing long term DIPC research projects. Among the local host community, there are also Ikerbasque researchers and Gipuzkoa Fellows, the latter being DIPC's star program in regard to attracting, retaining, and looking after scientific talent.

Collaboration Agreements

As a natural consequence of research collaborations already in place at DIPC, this year two formal agreements were signed with international centers in materials science.

Pedro Miguel Echenique and Juan Ignacio Cirac at the signing of the collaboration between the two institutions on January 16th at DIPC.

DIPC and the Max Planck Institute of Quantum Optics

January 16, 2015

The agreement signed between DIPC and the Max Planck Institute of Quantum Optics (MPQ) ratifies an already existing collaboration between the two centers. Its aim is to create new channels of exploration and deepen a continuing relationship. The recruitment and exchange of researchers between the centers is essential to inspire shared projects. The two centers will host scientific activities to further this exchange of knowledge. The agreement also seeks to develop innovative collaborations that combine lines of research in which DIPC and the MPQ are already leaders; condensed matter physics and quantum computing.

"The agreement is going to provide us with the necessary framework to put the existing collaboration on a firm footing and embark on new projects. At the MPQ we are convinced about the success of this cooperation."

Juan Ignacio Cirac
Director of MPQ

"Scientific collaborations are developed by persons, not institutions. These agreements have been signed not before but after actual collaboration. They emerge with content because researchers are already collaborating. The institutions add visibility by establishing a stable, long-term framework."

Pedro Miguel Echenique
President of DIPC

DIPC and the International Center for Materials Nanoarchitectonics (MANA)

August 27, 2015

MANA is a leading Japanese experimental research institute in nanotechnology that promotes the creation of a worldwide network of prestigious foreign partners as a way of achieving excellence. MANA is one of nine research centers sponsored by Japan's government as part of an ambitious program to support cutting-edge research based on internationalization, interdisciplinary domains and the excellence of the team of researchers. Thanks to the agreement DIPC joins this international nanoscience research network.

The purpose is to establish channels for cooperation and strengthen relations between the researchers of the two centers in order to develop joint innovative research projects in the field of materials science. The signature ceremony took place within the framework of the first Workshop MANA-DIPC (see page 123).

Pedro Miguel Echenique and Masakazu Aono at the signing of the collaboration between the two institutions on August 27th at DIPC.

"Our vision is to create a better future for humanity by opening up a new paradigm of nanotechnology through supporting the development of new materials. In order to achieve that, it is essential to have top-level international collaborators with shared interests, like DIPC."

Masakazu Aono
General Director of MANA

Science Communication

Events dedicated to intregrating science into our society

DIPC creates an open environment for science and society by cultivating an intellectual climate and enthusiasm for knowledge. The Science Communication program at DIPC establishes a fluid and permanent dialogue between science and society, and scientists and citizens. It helps to foster responsible social and scientific progress in a free and tolerant space that shows science is an accessible cultural activity for all — especially the coming generation of new scientists.

Seminars by Nobel Laureates and Distinguished Scholars

High-profile scientists and scholars are invited to DIPC to give a seminars and share their experiences with young researchers and the general public in an informal setting.

29/01/2015 **Iatrochemistry, cannabis and drug design**
Pilar Goya (Instituto de Química Médica CSIC, Madrid, Spain)

30/01/2015 **Landscape without neutrinos**
Juan José Gómez Cadenas (Instituto de Física Corpuscular CSIC-UV, Valencia, Spain)

18/03/2015 **La divulgación científica: un cuento inexacto**
Ana Montserrat Rosell (Director of TV program Tres14, RTVE, Spain)

06/10/2015 **La labor de la Fundación Española para la Ciencia y la Tecnología: Participación social en la ciencia**
José Ignacio Fernández Vera (General Director of FECYT, Spain)

22/10/2015 **Single-atom optical clocks**
David J. Wineland (Nobel Laureate in Physics 2012, NIST, Boulder, Colorado, USA)

15/12/2015 **100 años de relatividad general**
Alberto Galindo (Former President of the Royal Spanish Academy of Sciences, Spain)

Kutxa Lectures

The Kutxa Lectures started in 2010 and are organized in collaboration with Kutxa Obra Social in San Sebastian. Speakers include renowned scientists and Nobel laureates as well as science communicators and humanists working in the frontiers of science. This activity, addressed to citizens interested in science, has become an active part of the cultural life of the city of San Sebastian.

29/01/2015 **Paisaje con neutrinos**
Juan José Gómez Cadenas (Instituto de Física Corpuscular CSIC-UV, Valencia, Spain)

13/05/2015 **La imperfección de los modelos del clima**
Manuel Toharia Cortés (Scientific Director, The City of Arts and Sciences in Valencia, Spain)

24/06/2015 **How discoveries are made and why it matters**
John C. Polanyi (Nobel Laureate in Chemistry 1986, University of Toronto, Canada)
This lecture was part of the 15th International Conference on Vibrations at Surfaces (VAS15).

23/10/2015 **Quantum computers and Schrödinger's cat**
David J. Wineland (Nobel Laureate in Physics 2012, NIST, Colorado, USA)
Organized within the framework of the 2015 International Year of Light and Light-based Technologies.

top@DIPC Encounters. Zientziarekin solasean!

DIPC held the seventh edition of the annual Encounters between Nobel Laureates and leading researchers with high school students. The principal aim of these encounters is to foster students' interest in scientific and technological studies and to kindle a passion for knowledge in their young minds. In these informal encounters, prestigious invited scientists talk about their passion for science and research and answer questions from the students about their experiences throughout their lives and professional careers.

20/10/2015
Bizkaia Aretoa of the UPV/EHU, Bilbao
The guest researchers in this edition were:
David J. Wineland
(Nobel Laureate in Physics 2012, NIST, Colorado, USA)
Rafael Yuste
(New York City Mayor's Award for Excellence in Science and Technology 2002,
Columbia University, New York, USA)

More than **350 students and their teachers from 65 schools of Gipuzkoa, Bizkaia and Araba** participated at this year's Encounter. As usual, **Telefónica**, a long-time patron of DIPC, collaborates by giving an award to the most innovative, creative, original, surprising or interesting question.

For more information, visit:
www.topadipc.eu

Science Week

Once again DIPC, along with the Materials Physics Center and CIC nanoGUNE, participated at Science Week organized by the UPV/EHU. This year the stand and demonstrations were dedicated to nanostructures of different materials leading to amazing properties in the macroscale; the scale observable by the naked eye.

The joint program also included a comic and science workshop to create a short graphic story about a super-nano-hero with nanopowers.

05–07/11/2015
Museo San Telmo, Donostia/San Sebastián

Mestizajes

Besides traditional forms of knowledge, DIPC explores alternative spaces lying at the boundaries of different disciplines. Mestizajes is a trans-disciplinary program that bridges the gap between artistic, social and scientific branches of the humanities. Through a series of workshops, lectures, visits and collaborations, Mestizajes encourages people to take a critical look at reality from an innovative cutting-edge perspective. Projects such as, *Writer in Residence*, the play *The Interview*, and the biannual *International Meeting on Literature and Science* are carried out within this program.

24/04/2015
Museo San Telmo, Donostia/San Sebastián
Charla dedicada a las mujeres científicas
Marta Macho Stadler (UPV/EHU, Spain)
Part of a *Inspiraciencia*; literary contest with scientific inspiration.

18/03/2015
DIPC, Donostia/San Sebastián
La divulgación científica.
Un cuento inexacto
Ana Montserrat Rosell
(Director, Tres14, RTVE, Spain)

For more information, visit:
http://dipc.ehu.eus/mestizajes

On zientzia

On zientzia is a video contest organized yearly since 2010 by DIPC and Elhuyar Foundation, within the framework of the TV program *Teknopolis*. The aim is to promote the production and dissemination of short, original videos on science and technology subjects.

02/06/2015
The award ceremony took place at the headquarters of Donostia/San Sebastián 2016 European Capital of Culture.

Young Prize **Oroimena**
Mattin Zeberio (Student, 16 years old)

Best Video in Basque **Ideiak ukitzen**
David Muñoz (Teacher)

Best Video **La fuente de la juventud**
Abigail Rodríguez (Journalist, Canary Islands)

Special Mention **AXON pills**
Rosario Giménez (Chile)

In this fifth edition of On zientzia, 39 videos have participated, among them 16 within the Young Prize category, and 17 videos in Euskera.

For more information visit:
www.onzientzia.tv

High School Visits

During the 2015/2016 academic year, DIPC together with the Material Physics Center, continue the program of visits for groups of high school students. Both centers open their doors so these young students can meet researchers and view their work close up. This makes nanoscience and research real to them. Those who are considering a career in science are provided with guidance and encouragement. This year DIPC hosted a total of 381 students from 12 schools.

Activities in Bizkaia

DIPC is a Basque center, and it has a clear vocation to program outreach activities not only in Donostia/San Sebastián, but also in other cities across the Basque Country. This year we focused on Bilbao with two relevant public lectures:

20/10/2015
Bizkaia Aretoa of the UPV/EHU, Bilbao
El proyecto BRAIN y sus implicaciones para la ciencia, medicina y sociedad
Rafael Yuste
(New York City Mayor's Award for Excellence in Science and Technology 2002, Columbia University, New York, USA)

10/03/2015
Guggenheim Museum, Bilbao
From Matter to Life: Chemistry? Chemistry!
Jean-Marie Lehn
(Nobel Laureate in Chemistry 1987, ISIS, Université de Strasbourg, France)
Organized with the collaboration of Telefónica.

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DIPC HIGHLIGHT 2015

Effects of defects and water on perovskite solar cells

J.M. Azpiroz, E. Mosconi, J. Bisquert and F. De Angelis
Energy & Environmental Science 8, 2118-2127 (2015)

Perovskite is the structure of some minerals which have the general formula of ABX_3, where A and B are cations. This structure remained only as a tool for inorganic chemists and crystallographers to help them understand compounds until 2009, when it was found that $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ nanocrystals efficiently sensitize TiO_2 for the visible-light conversion in photoelectrochemical cells. Since then, the name perovskite has been associated to a new revolution in solar cells.

The efficiency of these solar cells have reached 20.1% in 2015, and has an efficiency limit of 31%, becoming a commercially attractive option.

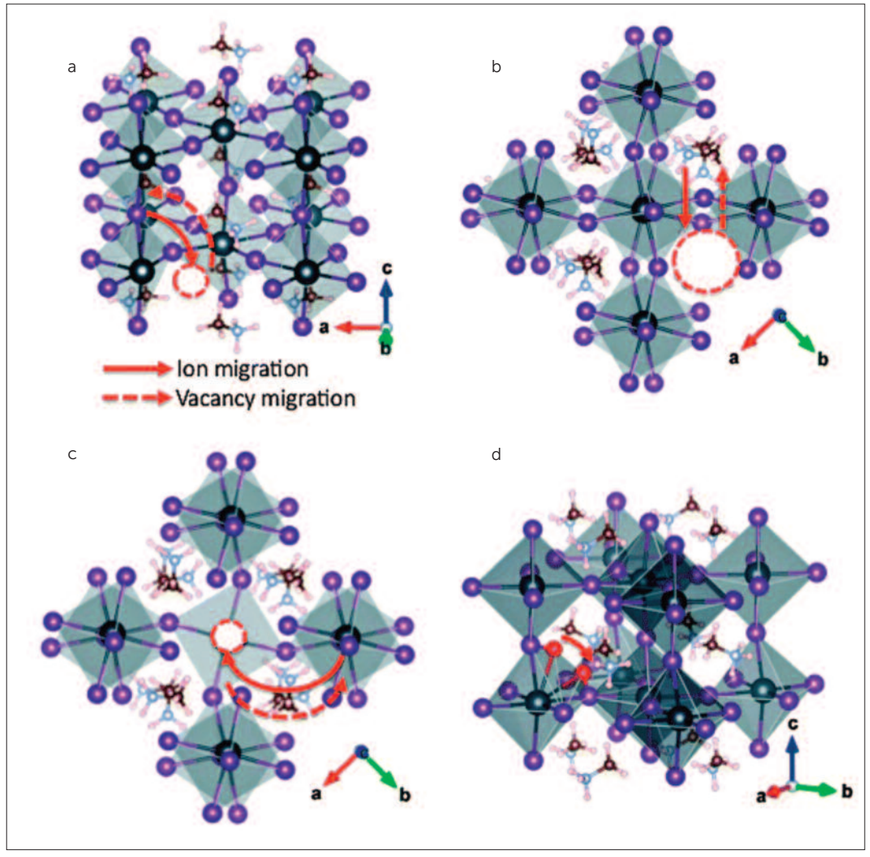
But, in order to increase the efficiency of perovskite solar cells some problems must be understood and solved. Azpiroz *et al* [1] first tackle some unusual findings which lack a proper theoretical explanation. What Azpiroz et al. did was a state-of-the-art first-principles computational analysis on realistic models of $MAPbI_3$ and $MAPbBr_3$ perovskites (MA = methylammonium), along with the crucial $MAPbI_3$ interface with TiO_2. They evaluated the migration energetics in tetragonal supercells, and, according to their calculations, the slow response typical in $MAPbI_3$ materials could be explained by the diffusion of MA or Pb vacancies. The identification of the mobile defects in perovskite solar cells, their migration across the perovskite material, and their effect on the operational mechanism of the device, may pave the way for the development of new solar cells with improved efficiencies.

Water may affect this kind of solar cells. Together with his colleagues, Azpiroz carried out *ab initio* molecular dynamics simulations to investigate the nature of the heterogeneous interface between water and the prototypical $MAPbI_3$ perovskite [2]. The results show that the effect of water depend on the surfaces. Thus, MAI- terminated surfaces are easily prone to solvation, while the PbI_2- terminated surface could act as a protective layer. In addition, a general band gap increase upon perovskite interaction with water with almost no changes in the tetragonal structure of the perovskite crystal was found.

This work, unraveling the atomistic details of the perovskite/water interface, may inspire new interfacial modifications and device architectures with increased stabilities, which could facilitate the widespread uptake of perovskite solar cells.

All in all, when new solar cells based on perovskites become commercially available, Ion Mikel Azpiroz (1986–2015) would somehow be there.

[1] J.M. Azpiroz, E. Mosconi, J. Bisquert and F. De Angelis. Defect migration in methylammonium lead iodide and its role in perovskite solar cell operation. Energy Environ. Sci. 8, 2118-2127 (2015).
[2] E. Mosconi, J. M. Azpiroz, and F. De Angelis. *Ab Initio* Molecular Dynamics Simulations of Methylammonium Lead Iodide Perovskite Degradation by Water. Chem. Mater. 27 (13), 4885–4892 (2015).



Diffusion paths defects (a-d). Vacancies are highlighted with dashed circles. Red atoms refer to interstitial defects. Solid lines stand for the migration of the ions, whereas dashed lines indicate the trajectory of the vacancy. White = H, brown = C, blue = N, purple = I, and black = Pb atoms.

Ion Mikel Azpiroz Apezetxea recently passed away.
His colleagues and friends at the Theoretical Chemistry Group at UPV/EHU and DIPC want to dedicate these lines to his memory.

Ion Mikel, good friend,
you will be in our hearts forever.

DIPC HIGHLIGHT 2015

Atomistic near-field nanoplasmonics: Reaching atomic-scale resolution in nanooptics

M. Barbry, P. Koval, F. Marchesin, R. Esteban, A. G. Borisov, J. Aizpurua, and D. Sánchez-Portal
Nano Letters 15 (5), 3410–3419 (2015)

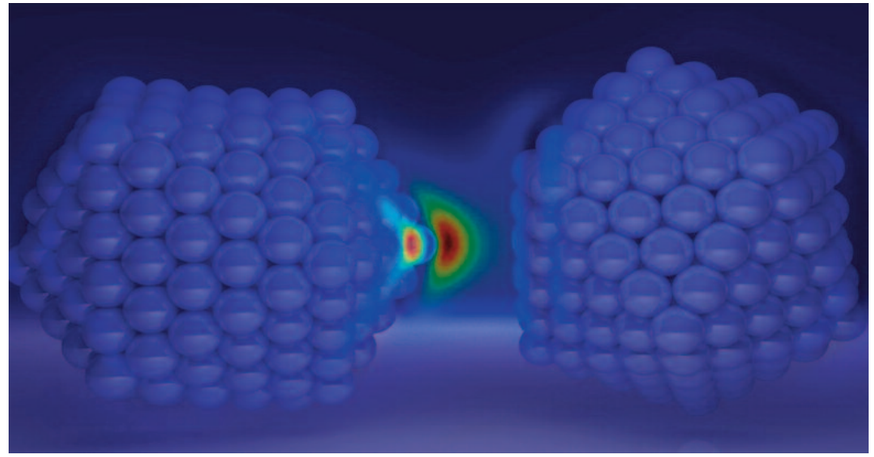
The electromagnetic fields of antennae are not the same far from the antenna (far-field) than close to them (near-field). While the far field is the region where we find a "normal" electromagnetic radiation, dominated by electric-dipole type electric or magnetic fields, the near field is governed by multipole type fields, which can be considered as collections of dipoles with a fixed phase relationship. The boundary between the two regions depends on the dominant wavelength emitted by the antenna. Moreover in the far-field region of an antenna, radiation decreases as the square of distance, and absorption of the radiation does not feed back to the transmitter. However, in the near-field region, absorption of radiation does affect the load on the transmitter.

If this is true for macroscopic antennae, in the nano-world, where we are dealing with sizes very close to those of molecules, the application of the standard procedures involving the Maxwell equations to study the optical response of a nano-system seems unfit the closer we come to atomic-scale. Still, these procedures are applied.

Now a group of researchers, led by Javier Aizpurua and Daniel Sánchez-Portal from the Materials Physics Center (CSIC/EHU) and DIPC, study the optical response of plasmonic nanoparticles and, using sodium clusters as an example, show that the atomistic details of the nanoparticles morphologies determine the presence of a peculiar near-field. The results, published in Nano Letters, provide new insights into the limits of what can be done optically at the nano-scale, with important applications in the optical resolution of field-enhanced spectroscopies and microscopies.

When an object has an electrical charge, its electric fields are strongest at the sharpest features of that object. For example, electric fields are strongest at the sharp tip of a lightning rod. This phenomenon also occurs at the nanoscale, where particles of metals such as gold or silver can produce oscillating electric fields when irradiated by particular wavelengths of light (plasmon resonance). Using time-dependent density functional theory and performing atomistic quantum mechanical calculations of the optical response of plasmonic nanoparticles and its dimers, this work shows how the atomic features at the surfaces of plasmonic nanoparticles do localize electromagnetic fields down to atomic-scale dimensions showing resonant (plasmonic) and non-resonant (lightning rod effect) field enhancements that alter the standard conception of plasmonic fields' localization.

Electromagnetic field localization in nanoantennas is one of the leitmotivs that drives the development of plasmonics



Model of a nanometric plasmonic cavity formed by two sodium clusters containing 380 atoms. In this case, a protruding tip from one of the clusters confronts a planar facet from the other particle. A cut of the intensity of the induced electromagnetic field at the resonance frequency of the cavity is shown in a contour plot. Black and red correspond to the largest intensities. As clearly seen, the near field localizes onto a spot of atomic dimensions close to the tip. Due to this effect the maximum field enhancement in this cavity is twice as large as that found in a cavity formed by two planar facets. This can have important consequences in several areas, including tip enhanced microscopies.

The atomistic details of the nanoparticles morphologies determine the presence of subnanometric near-field hot spots

The results indicate that, at the vertices and edges formed at the contact of different crystalline facets, it is possible to localize plasmons with subnanometric resolution and beat the typical plasmonic confinement imposed by the nanoparticle size. Such sensitivity to the atomic details of a structure could explain the lack of reproducibility between apparently similar experiments, but could also provide a root for further optimization of morphologies. This hints to the atomic-scale structure of plasmonic interfaces becoming a new area of research as it will likely be relevant to allow superresolution in a variety of experimental near-field techniques.

Density of trap states and auger-mediated electron trapping in CdTe quantum-dot solids

S.C. Boehme, J.M. Azpiroz, Y.V. Aulin, F.C. Grozema, D. Vanmaekelbergh, L.D.A. Siebbeles, I. Infante, and A.J. Houtepen
Nano Letters 15, 3056–3066 (2015)

Minimizing losses in any kind of electronic device is always important, but it is paramount in nanoelectronics. Still, most of the phenomena that lead to inefficiencies in the operation of these nanodevices are poorly understood.

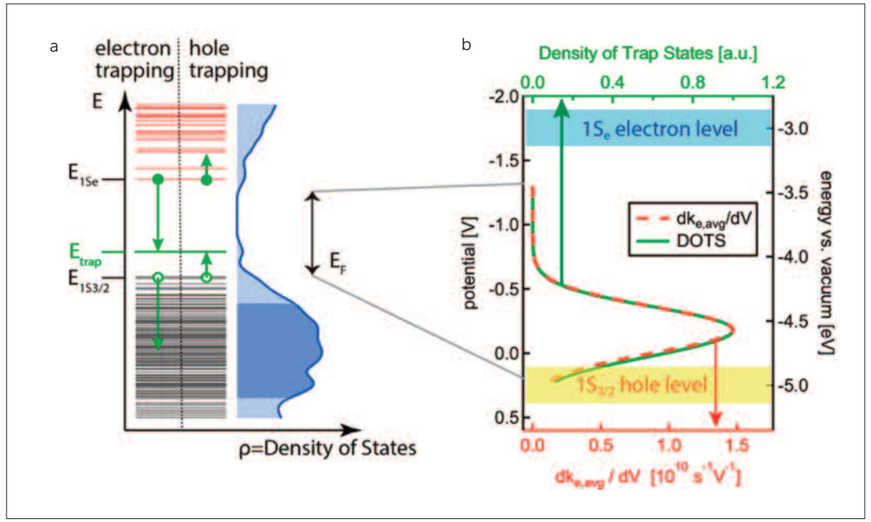
That is the case in quantum dots based devices such as solar cells, LEDs, and thermoelectrics, where a major limitation to the efficiency is charge trapping. Although empirical approaches led to a reduction of trapping and thereby efficiency enhancements, the exact chemical nature of the trapping mechanism remains largely unidentified. In devices made of crystalline bulk materials, the most common trapping sites are impurities or defects of the crystal structure such as vacancies or interstitial atoms. However, in multi- and nanocrystalline materials, surface defects play a dominant role. A quantum dot (QD) is a nanometric crystalline structure of semiconductor materials. In a QD, electrons are confined in a region of space, thus creating a well-defined structure of energy levels that depends very much on the size and shape of the quantum dot.

Now, a group of researchers that include Jon Mikel Azpiroz and Ivan Infante from the Kimika Fakultatea UPV/EHU and DIPC, has focused on a quantum-dot cadmium telluride solid to investigate both experimentally and theoretically the trapping mechanism and the kind of chemical reaction at play during charge trapping in the quantum dots. Their results are published in *Nano Letters*.

The researchers report the first experimental determination of the density of trap states of a film of cadmium telluride quantum dots, using a novel combination of electrochemistry and ultrafast spectroscopy. When traps are empty, electron trapping proceeds on a (sub-)picosecond time scale; when traps are filled electrochemically, this process takes nanoseconds. They find a density of trap states close to the valence band. The theoretical calculations done using density functional theory are consistent with this finding and assign it to dicoordinated tellurium atoms at the quantum dot surface as a result of a loss of ligands during the film processing.

Time-resolved photoluminescence experiments reveal that hole trapping also occurs, albeit at least one order of magnitude slower than electron trapping. The slower hole trapping and the fast capture of electrons by traps close to the valence band can be explained by an Auger-mediated trapping mechanism (see figure).

In all, the researchers are able to assign a density of trapping states to the exact composition and geometry of the surface using a unique combination of experimental and theoretical approaches, identifying the bottlenecks for improving quantum-dot based devices.



(a) Schematic of Auger-mediated electron and hole trapping to a trap state at the QD surface, at an energy close to the valence band edge. Assuming the matrix elements for electron and hole Auger mediated trapping do not differ too much, electron trapping proceeds faster due to a larger density of acceptor states for the scattered hole (deep in the valence band) compared to a sparser density of acceptor states for the scattered electron (close to the conduction band edge). The occupied and unoccupied molecular orbitals (gray and red horizontal bars, respectively) and the density of states (light blue shaded area) were obtained from DFT calculations. The dark blue shaded area depicts the hole acceptor states for the range of Fermi levels within the experimental probe window (double-headed arrow). (b) Derivative of the average electron trapping rate constant (red dashed line) and density of trap states (green solid line).

A deeper understanding of charge trapping is necessary to advance the science and application of QDs.

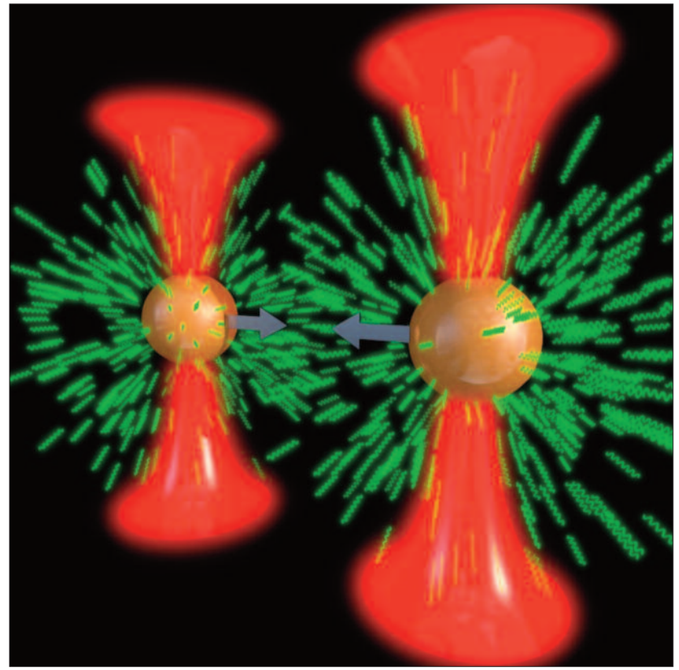
Controlling dispersion forces between small particles with artificially created random light fields

G. Brügger, L.S. Froufe-Pérez, F. Scheffond, and J.J. Sáenz
Nature Communications 6, 7460 (2015)

Dispersion forces between molecules arise from electromagnetic fields generated by natural quantum and thermal fluctuations. In an article appearing in *Nature Communications* the groups of Prof. Scheffold in Fribourg (Switzerland) and Prof. Sáenz in Madrid and Donostia/San Sebastian (Spain) show that dispersion forces can be induced, controlled and tuned by random laser fields.

van der Waals forces are ubiquitous in nature and responsible of uncountable natural processes like adhesion or surface tension and play a key role in the behaviour observed in biological fluids (proteins, blood cells, ...), paints, inks or foodstuffs. A team of researchers from the Donostia International Physics Center (DIPC), Condensed Matter Physics Center (IFIMAC-UAM) and Fribourg University show for the first time that it is possible to induce and control this type of dispersion forces at the nanoscale with external random laser fields.

The origin of van der Waals forces, also known as "dispersion forces", can be found in naturally present, extremely fast fluctuating electric and magnetic fields. Compared to ordinary chemical bonds, such fluctuations induce a relatively weak interaction between molecules and small objects. However, by combining the van der Waals forces of millions of small hairs, geckos and some spiders (including Spiderman) can adhere to a surface being able to climb vertical smooth walls without any adhesive.
To mimic the natural field fluctuations (of both quantum and thermal origin), the researchers generated a laser light cloud with properties similar to the light you see when the sun shines through mist on a foggy day, albeit with a much higher intensity. In the experiment two tiny plastic beads are held in place and embedded in the light cloud (see figure). The interaction force between the beads can be measured by studying precisely the relative position of the two particles with a microscope.



Two tiny plastic beads are held in place and embedded in the light cloud.

Emulating Spiderman: adhesion forces activated by laser light clouds

The higher the light intensity in the cloud, the more the two particles attract each other. Like in nature, the forces only depend on the relative distance between the particles, but not their actual position within the cloud. The strength and properties of the forces present can also be controlled by the appropriate selection of the intensity and the colour of the light in the cloud.

The results suggest that it should be possible to completely control interactions between small bodies in two or three dimensions. This approach could facilitate the design of colloidal suspensions and nanostructured materials with tailored properties "à la carte".

Spatial variation of a giant spin-orbit effect induces electron confinement in graphene on Pb islands

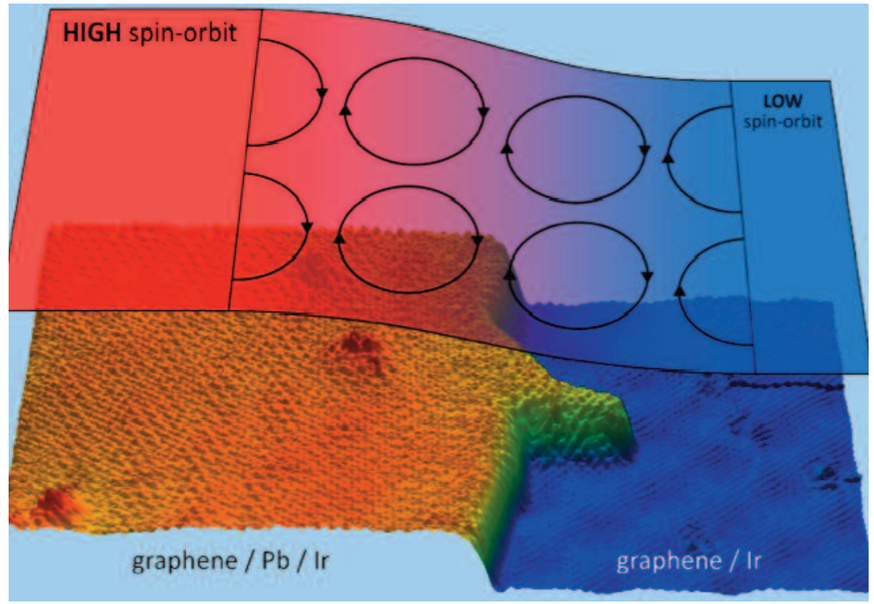
F. Calleja, H. Ochoa, M. Garnica, S. Barja, J.J. Navarro, A. Black, M.M. Otrokov, E.V. Chulkov, A. Arnau, A.L. Vázquez de Parga, F. Guinea, and R. Miranda
Nature Physics 11, 43-47 (2015)

When lead atoms are intercalated in a graphene sheet, the electrons behave as if they felt a powerful magnetic field. This effect is due to the strong interaction of the electrons' spin with their orbital motion that appears because graphene electrons "feel" the proximity of lead atoms. Paraphrasing Albert Fert, 2007 Nobel Prize in Physics, it is a type of spin-orbitronics. This is a novel direction of spintronics, an emerging technology promoted by the European Union to create advanced computational systems.

Graphene has been considered the material of the future due to its extraordinary mechanical, optical, and electronic properties, like its high electron mobility. However, pristine graphene does not show magnetic properties and, so far, no definitive method has been found to manipulate its electrons (or any of their properties) to use it in new magneto-electronic devices.

Now, it seems that there is a key to do it: the intercalation of Pb atoms forming several nm wide islands below the sea of graphene electrons. As a consequence of the proximity of Pb atoms, an increase of the spin-orbit interaction of graphene electrons takes place. To obtain this effect, one needs to evaporate lead atoms on top of a graphene layer grown on an iridium crystal. Under certain conditions, lead atoms form 'islands' between the graphene layer and the top most Ir atomic layer, after having diffused across the graphene layer. In this way, the pristine graphene electrons in π-bands close to the Fermi level behave as if they felt a magnetic field, which facilitates the selective control of the flow of spins.

A consequence of this finding is that graphene could be used as an active component in a new generation of devices based on the use of the electron spin degree of freedom within the new technology called spintronics that started with the discovery of giant magnetoresistance (GMR). This finding, for which Peter Grünberg and Albert Fert were jointly awarded with the 2007 Nobel Prize in Physics, is an effect that causes great changes in the electric resistance of fine multi-layer materials and has led to the development of components as varied as the reader heads on hard disks or the sensors in *airbags*.



In the sea of graphene (over an iridium crystal), electrons' spin-orbit interaction is much lower than that created by intercalating a Pb island. (Image: IMDEA Nanoscience, UAM, ICMM-CSIC, CFM –CSIC-UPV/EHU– and DIPC)

Graphene with intercalated lead atoms could be used as an active component in a new generation of magneto-electronic devices

The first generation of spintronic or magnetoresistant devices was based on the effect that magnetic materials have on electron spin. But a second generation is already up and running, and encompasses this new study, in which electrons' own spin-orbit interaction acts on them as if there were a real external magnetic field, even if there is not any. Scientists' final goal is to willfully control the type of spin the electrons in this new material have in order to apply it to the electronic devices of the future.

Sulfur-bridged terthiophene dimers: How sulfur oxidation state controls interchromophore electronic coupling

C.D. Cruz, P.R. Christensen, E.L. Chronister, D.Casanova, M.O. Wolf, and C.J. Bardeen
Journal of the American Chemical Society 137, 12552–12564 (2015)

A great deal of work has been focused on synthesizing electron donor/acceptor pairs to mimic the efficient natural light harvesting systems. The most common approach is to unite an electron-rich donor with an electron-deficient acceptor using a π-conjugated linkage or "bridge". Separation of the donor and acceptor by such a bridge can enable charge transfer over large distances, limiting charge recombination. While remarkable photovoltaic performance has been achieved using this approach, these asymmetric systems only partially mimic the naturally occurring photosynthetic reaction centers, where symmetric chromophore pairs have a central role in controlling excited-state dynamics.

The rational design of symmetrically bridged chromophore dimers, also called bichromophores, has attracted considerable theoretical and practical interest. For example, bichromophoric systems have also found applications in organic light emitting diodes (OLEDs) and high-efficiency blue OLEDs were fabricated using SO_2-bridged symmetric bichromophores.

atom results in systematic enhancement of the photoluminescence by oxidizing the bridging sulphur. These experiments were done using terthiophenes as chromophores.

The observation that simply linking two terthiophenes together via a sulphur atom could lead to new charge transfer excited states and increase the photoluminescence yield raised several questions regarding the origin of the changes in spectroscopic behavior.

As this class of sulphur-bridged terthiophene dimers, with potential applications in organic electronics, provides an ideal model system in which to study fundamental questions about the excited-state behavior in symmetric bichromophore systems, a group of researchers, including David Casanova, an Ikerbasque Research Fellow working at the Chemistry Faculty of UPV/EHU and DIPC, focused on answering this questions and combined spectroscopy and computation to obtain a comprehensive picture of the photodynamics of sulphur-bridged terthiophene dimers. The results are published in the *Journal of the American Chemical Society*.

The researchers used optical spectroscopy and electronic structure theory to develop a complete picture of the photophysics of a group of terthiophene derivatives (Figure 2). They found that the bridge itself does not significantly affect the excited-state structure, but the oxidation state of the sulphur bridge mediates the amount of electronic coupling between the two terthiophene chromophores.

Based on computational results, the researchers propose a mechanism in which electrostatic screening by lone pairs on the sulphur linker controls the charge transfer character of the excited-state wave function. This suggests that it is possible to use electron density on the bridge to mediate intramolecular interactions and tune the electronic coupling between identical chromophores without altering the dimer geometry or solvent polarity.

These results not only reveal the origins of the novel properties of a specific class of terthiophene bichromophores but also provide new directions for the design of symmetric chromophore systems that may find applications in fields ranging from artificial photosynthesis to organic electronics.

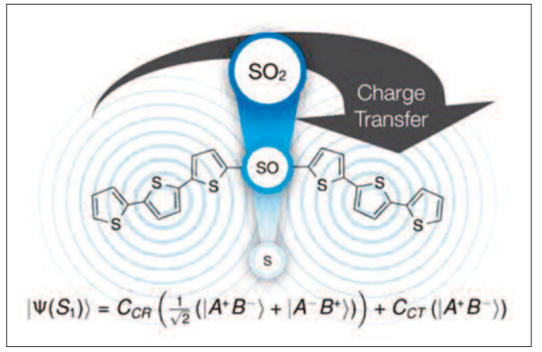


Figure 1: Controlled electronic coupling.

Mimicking Nature's light-harvesting efficiency

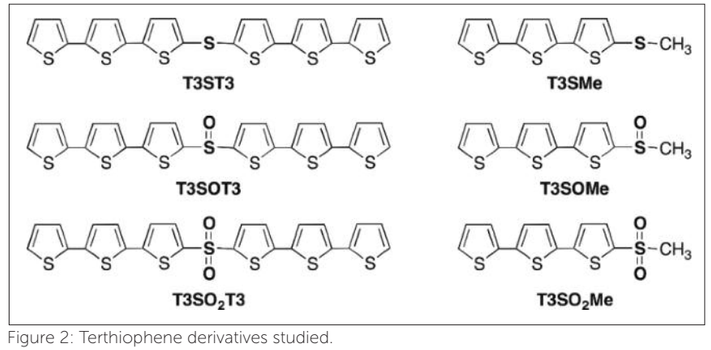


Figure 2: Terthiophene derivatives studied.

DIPC HIGHLIGHT 2015

High-pressure hydrogen sulfide from first principles: A strongly anharmonic phonon-mediated superconductor

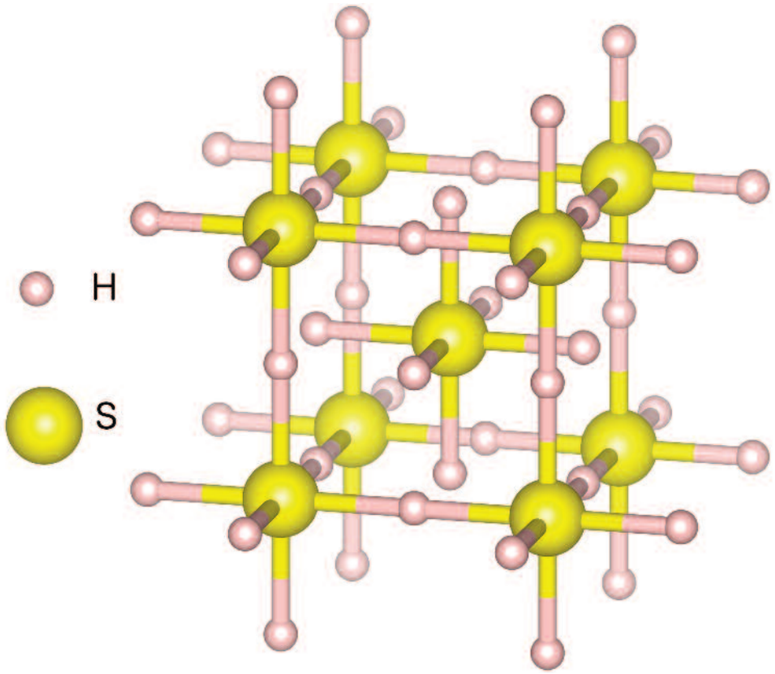
I. Errea, M. Calandra, C.J. Pickard, J. Nelson, R.J. Needs, Y. Li, H. Liu, Y. Zhang, Y. Ma, and F. Mauri
Physical Review Letters 114, 157004 (2015)

Scientists from the Donostia International Physics Center (DIPC) in collaboration with researchers from France, England, Canada and China use first-principles calculations to explain the origin of the newly discovered record superconductivity in high-pressure hydrogen sulfide. The outstanding value of the superconducting critical temperature is explained by the coupling of electrons with extremely anharmonic lattice vibrations.

Achieving room temperature superconductivity is among the most pursued but elusive goals of scientists. Despite the discovery three decades ago of high-temperature superconductivity in the cuprates raised enormous hopes, the maximum value for the superconducting critical temperature achieved in these materials was 164 K. Recently, a team or researchers claimed to have observed superconductivity as high as at 190 K in high-pressure hydrogen sulfide, breaking all the records thus far. The theoretical work by Ion Errea, researcher from DIPC, and collaborators, demonstrates that, instead of an unknown coupling mechanism as in the cuprates, the interaction between the electrons and the lattice vibrations (the phonons) drives the superconducting transition in hydrogen sulfide. These results, published in the prestigious *Physical Review Letters* journal as an *Editor's Suggestion*, show that high-temperature superconductivity can be attained within conventional electron-phonon superconductors.

In the first place the researchers studied the stability and possible decomposition of hydrogen sulfide (H_2S). The conclusion is that H_2S, which is stable at ambient conditions, is not a stable compound at high pressure, and decomposes producing HS_2 or H_3S. While the HS_2 compound yields superconducting transition temperature (T_c) of around 30 K, far from the experimental observation, the H_3S compound, which crystallizes in the cubic structure shown in the figure, has a huge electron-phonon coupling that might explain the outstanding measured value for T_c. However, the observed critical temperature can only be explained if anharmonic effects are taken into account in the description of the phonons. Indeed, due to the presence of very light hydrogen atoms that vibrate with a large amplitude around their equilibrium positions, anharmonicity has a huge impact on the phonon spectra. Thus, the researchers conclude that the record high-temperature superconductivity observed in hydrogen sulfide is due to the large interaction between electrons and anharmonic phonons.

Room temperature superconductivity among the most pursued but elusive goals of scientists



Crystal structure of superconducting H_3S.

Unveiling the Origin of the Record Superconductor in high-pressure hydrogen sulfide

DIPC HIGHLIGHT 2015

Nanoscale origin of mesoscale roughening: Real-time tracking and identification of three distinct ruthenium oxide phases in ruthenium oxidation

J.I. Flege, B. Herd, J. Goritzka, H. Over, E.E. Krasovskii, and J. Falta
ACS Nano 9, 8468 (2015)

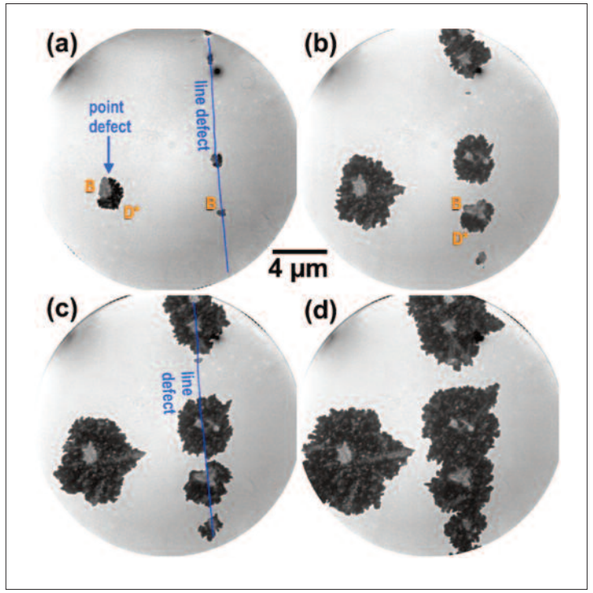
Oxidation is a ubiquitous phenomenon that proceeds via the electrochemical interaction of ambient oxygen molecules with atoms of the metal. Fundamentally, the oxidation of metal surfaces represents a remarkably complex reaction scenario at the solid-gas interface, in which heterogeneities at the surface as well as the supply and transport of the reacting surface species, are decisive ingredients.

In the course of metal oxide formation, the metal-metal bonding is replaced by metal-oxygen bonding, a process that depends heavily on temperature and that determines the reaction rate at low temperatures. Even if the initial processes in the oxidation of a metal surface are well understood on the microscopic level, the further growth of the oxide is frequently accompanied by a substantial roughening and patterning of the surface at the mesoscale, whose physical and chemical origin is far less understood. However, this information is critical if we are to understand catalysis properly; even more if we consider that recent studies hint that metal oxides could be more active than the current metal catalysts.

To achieve this what is needed is a non-destructive laboratory method that would allow to map the mesoscale surface morphology and structure on a few nanometer scale. This is exactly what a group of researchers, including Ikerbasque Prof. Eugene Krasovskii from the Materials Physics department (UPV/EHU) and DIPC, has provided with a proof-of-principle testing of the oxidation of a ruthenium surface at high temperatures using intensity-voltage low energy electron microscopy, I(V)-LEEM. This approach, when combined with state-of-the-art theoretical models built from ab initio scattering theory, yields a real-time structural identification in a reactive environment. The results are published in ACS Nano.

Above temperatures of 550 K, the initial oxidation of Ru(0001) has been shown by scanning tunneling microscopy (STM) to proceed via a modified nucleation and growth mechanism. However, closer inspection of the available STM images in the literature reveals the presence of unknown surface components that seem to coexist with the established RuO_2(110) phase, rendering the oxidation of the Ru(0001) system more complex than frequently anticipated.

An in situ electron reflection method demonstrates that the RuO_2(100) phase grows first and then fosters the nucleation of other faces of RuO_2



LEEM time-lapse sequence showing the oxidation of the Ru(0001) surface by exposure to O_2.

In the present work, the researchers used a combination of I(V)-LEEM and micro-diffraction analysis to identify emerging ruthenium oxide phases as the (110), (100), and (101) orientations of RuO_2. By comparing to ab initio calculations of electron scattering from crystalline surfaces, the pronounced differences found in the I(V)-LEEM curves at very low energies were traced back to the unoccupied electronic structure of the differently oriented RuO_2 crystallites. This correspondence allows to follow the nucleation, growth and coalescence of different faces of the same nanocrystalline oxide in real-time.

Most importantly, this methodology also enables real-time kinetic studies of dynamic processes in complex catalytic materials under reaction conditions.

Very large thermophase in ferromagnetic Josephson junctions

F. Giazotto, T.T. Heikkila, and F.S. Bergeret
Physical Review Letters 114, 067001 (2015)

The concept of thermophase refers to the appearance of a phase gradient inside a superconductor originating from the presence of an applied temperature bias across it. In this work we investigate the thermoelectric response of a thermally biased Josephson junction based on a ferromagnetic insulator and predicts the occurrence of a very large thermophase. This effect could be of strong relevance in thermometry and radiation sensing.

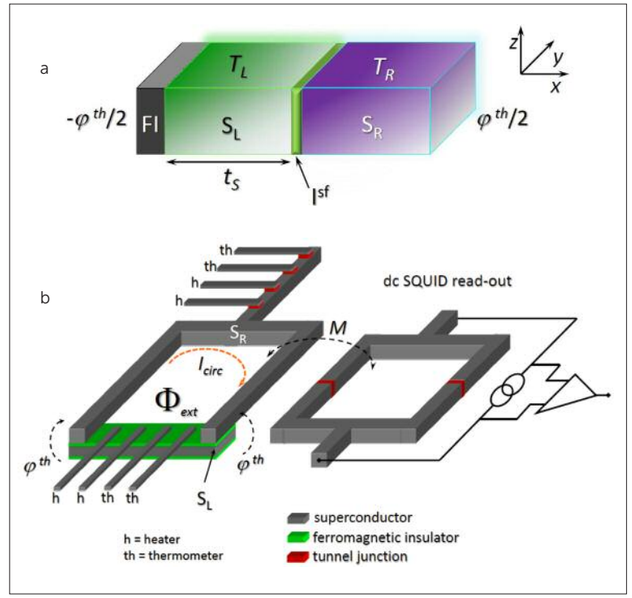
When a thin layer of an insulating material is sandwiched between two identical superconductors, and this layer is thin enough, correlated electron pairs can tunnel from one superconductor to another. This leads to a non-dissipative current through the junction that depends on the difference between the phases in the two superconducting electrodes. The existence of this "supercurrent" through this type of junctions was first predicted by Brian Josephson in 1969, and it is now known as the Josephson effect.

The Josephson effect and the Josephson junction have found multiple applications in quantum-mechanical circuits, like superconducting quantum interference device (SQUIDs), superconducting qubits, and rapid single flux quantum (RSFQ) digital electronics.

A group of researchers, that includes Sebastián Bergeret from the Materials Physics Center (CSIC-UPV/EHU joint center) and DIPC, have addressed the long-standing question of whether a temperature gradient between two superconductors can lead to an analog to the Josephson effect. The result of this research is a work published in *Physical Review Letters* that predicts the appearance of a huge thermophase when there is a temperature difference between the superconducting electrodes separated by a ferromagnetic insulator. This effect is several orders of magnitude larger than the one predicted to occur in conventional Josephson junctions.

The concept of thermophase refers to the appearance of a phase gradient inside of a superconductor due to a temperature gradient across it. As mentioned above, phase differences in superconductors are associated with supercurrents. In the presence of a temperature gradient these supercurrents may counterbalance the induced quasiparticle currents preventing the formation of any voltage drop across the superconductor.

In the case of the junction shown in the figure, the total electric current flowing through the junction is the result of the sum of the quasiparticle and the Josephson contributions. In an electrically open configuration (no closed circuit) the total charge current has to vanish. This implies that the quasiparticle and



(a) Sketch of a generic S-FI-I-S Josephson junction discussed in the text. It consists of two identical superconductors, SL and SR, tunnel coupled by a ferromagnetic insulator FI and a nonmagnetic barrier I.

(b) Scheme of a detection setup consisting of a temperature-biased superconducting quantum interference device (SQUID) based on the previous junction.

Such junctions are potentially attractive for ultrasensitive radiation-sensing and thermometry applications

Josephson contributions have to cancel each other. This cancellation is the origin of the thermophase as the Josephson contribution depends on the phase difference. Thus, the thermophase (the phase difference at which the cancellation occurs) is a measure of the amplitude of the thermoelectric effect at the contact between superconductors.

In this work, Sebastian Bergeret and collaborators demonstrate that the inclusion of a ferromagnetic insulator may lead to a very large thermophase that can reach $\pi/2$ across the contact for suitable temperatures and structure parameters. In order to assess experimentally their prediction, they propose a realistic setup realizable with state-of-the-art nanofabrication techniques and well-established materials, based on a superconducting quantum interference device (see Figure). This sharp thermophase response combined with the low heat capacity of superconductors could be used to build ultrasensitive thermometers and radiation detectors, where the radiation induced heating of the superconductors is detected via the thermophase [1].

[1] F. Giazotto, P. Solinas, A. Braggio, and F.S. Bergeret. Ferromagnetic-Insulator-Based Superconducting Junctions as Sensitive Electron Thermometers. *Phys. Rev. Applied 4*, 044016 (2015).

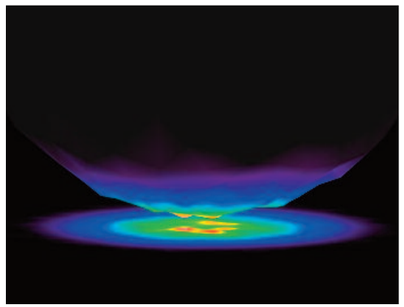
Radiative heat transfer in the extreme near field

K. Kim, B. Song, V. Fernández-Hurtado, W. Lee, W. Jeong, L. Cui, D. Thompson, J. Feist, M.T.H. Reid, F.J. García-Vidal, J.C. Cuevas, E. Meyhofer and P. Reddy
Nature 528, 387-391 (2015)

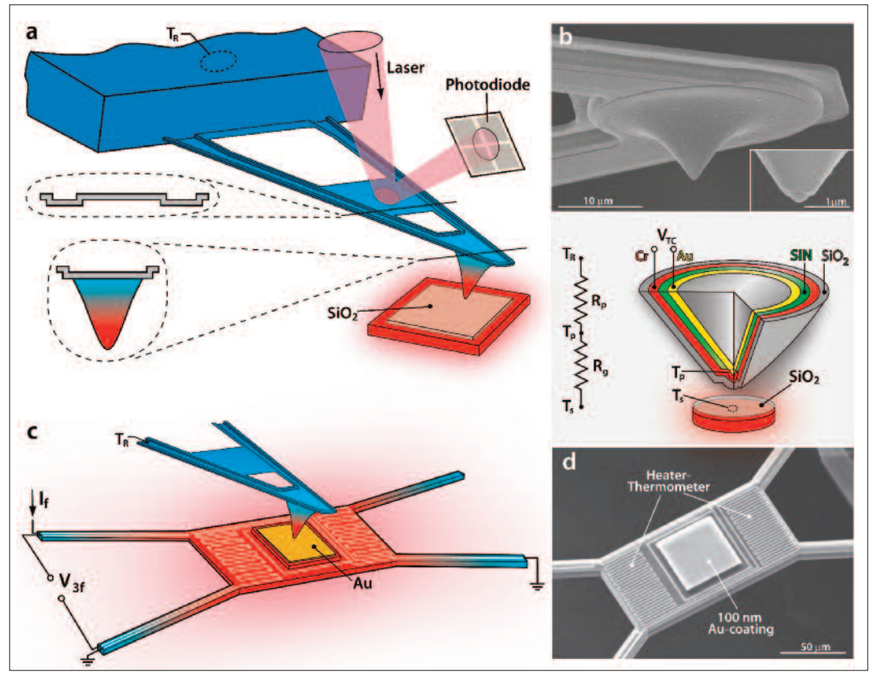
Radiative heat transfer between objects at different temperatures is of fundamental importance in applications such as energy conversion, thermal management, lithography, data storage, and thermal microscopy.

It was predicted long ago that when the separation between objects is smaller than the thermal wavelength, which is of the order of 10 μm at room temperature, the radiative heat transfer could be greatly enhanced over the theoretical limit set by the Stefan-Boltzmann law for blackbodies. This is possible due to the contribution of the near field in the form of evanescent waves (or photon tunneling). In recent years, different experimental studies have confirmed this long-standing theoretical prediction. However, and in spite of this progress, recent experiments exploring the radiative thermal transport in nanometric gaps have seriously questioned our present understanding of thermal radiation at the nanoscale. In particular, these experiments cast some doubt on the validity of *fluctuational electrodynamics*, which is presently the standard theory for the description of near field radiative heat transfer (NFRHT).

This fundamental puzzle has now been resolved in a work published in *Nature* by a collaboration between different groups at the Universidad Autónoma de Madrid, University of Michigan and MIT, in which Prof. Francisco J. García-Vidal, frequent visitor of DIPC has been involved. In this work, the authors used a novel type of scanning thermal probes with embedded thermocouples to measure the NFRHT between different materials (dielectrics and metals) down to gaps as small as 2 nm. In particular, it is shown how heat transfer between silica-silica, silicon nitride-silicon nitride and gold-gold surfaces exhibits a dramatic enhancement as the gap is reduced down to a few nanometers. Moreover, they have presented state-of-the-art simulations of the radiative heat transfer in the framework of fluctuational electrodynamics theory that were able to reproduce all the experimental observations without any adjustable parameter. These results unambiguously demonstrate that fluctuational electrodynamics based on Maxwell equations provides an accurate description of the NFRHT between both metals and dielectrics all the way down to nanometer-size gaps. This work clarifies the fundamental mechanisms that govern the radiative heat transfer at the nanoscale and it establishes a firm basis for the future design of novel technologies that make use of nanoscale radiative heat transfer.



Distribution of the radiative heat transfer between a SiO_2 AFM tip and a SiO_2 substrate separated by a few nanometers.



Experimental setup and Scanning Electron Microscope (SEM) images of SThM probes and suspended microdevices. a, Schematic of the experimental setup where a SThM probe is in close proximity to a heated substrate (inset shows the cross-section of the SThM probe). The scenario for SiO_2 measurements is shown (the coating on the substrate is replaced with SiN and Au in other experiments). **b**, SEM image (top panel) of a SThM probe. The inset shows a SEM image of the hemispherical probe tip, which features an embedded Au-Cr thermocouple. The bottom panel shows a schematic cross-section for a SiO_2-coated probe employed in SiO_2 measurements. For SiN and Au measurements the outer SiO_2 coating is appropriately substituted as explained in the SI. A resistance network that describes the thermal resistance of the probe (R_P) and the vacuum gap ($R_g = (G_{eNFRHT})^{-1}$) as well as the temperatures of substrate (T_S), tip (T_P) and reservoir (T_R) is also shown. **c**, Schematic showing the measurement scheme employed for high resolution eNFRHT measurements of Au-Au. The amplitude of the supplied sinusoidal electric current is I_f, the sinusoidal temperature oscillations at 2_f are related to the voltage output V_{3f}. **d**, SEM image of the suspended microdevice featuring the central region coated with Au and a serpentine Pt heater-thermometer.

Active quantum plasmonics

D.C. Marinica, M. Zapata, P. Nordlander, A. K. Kazansky, P.M. Echenique, J. Aizpurua, and A.G. Borisov
Science Advances 1, e1501095 (2015)

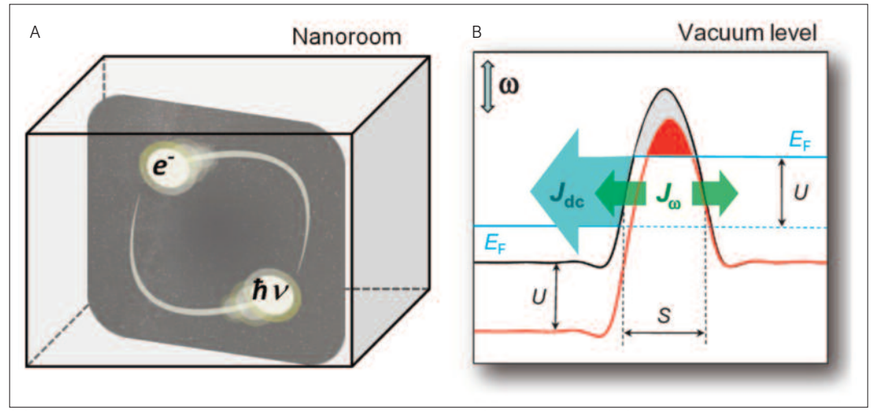
The exchange of information between photons of light and electrons in miniaturized electronic devices is a longstanding challenge that might be now closer to a solution thanks to the proposal presented by a team of researchers in an international collaboration at the Center for Materials Physics (CSIC-UPV/EHU) and Donostia International Physics Center (DIPC) in San Sebastian (Spain), the Institute of Molecular Sciences in Orsay (France), the University of Los Andes (Colombia) and the Nanophotonics Laboratory in Houston (USA).

Controlling light with electrical DC (static) currents at the nanoscale

Light is a fast and reliable means of delivery information which is currently used in modern communications, however, most of this photonic information has to be processed and dealt with by electrons in miniaturized electronic devices, such as in state-of-the-art transistors. Due to the mismatch of dimensions and speed of one (photon) and another (electron), a problem arises when transferring information from the photons of light to the electrons in electronic devices, and vice versa. The electrical fields associated with a photon oscillate very fast in time (of the order of 1015 times per second) and spread in space due to the diffraction limit, whereas electrons typically move driven by constant, static fields in much more reduced dimensions of a few nanometers. This impossibility for electrons and photons to talk to each other in reduced dimensions is a current technological bottle neck.

Now, the international research team makes a conceptual proposal where the quantum tunneling regime in a metallic nanogap, which can be seen as a metallic "nanoroom", is predicted to serve as a matching environment to facilitate the dialogue between photons and electrons, exchanging information in a fast and effective way. In this miniaturized "nanoroom", on the one hand, photons are squeezed down to the same nanoscale dimensions as those typical of electrons, thanks to a collective excitation of the material, the so-called plasmon. Plasmons help to "trap" light in this "reduced room". On the other hand, the excitation of this "trapped light" is found to depend on the actual DC (static) current driven between the two electrodes of the "nanogap room", thanks to the tunneling of electrons between one wall of the room and the other wall.

Photons and electrons talk to each other in a tiny room



(A) Schematics of a figurative nanoroom where photons (ħν) and electrons (e-) are trapped establishing a dialogue to transfer information. The nanoroom is a plasmonic nanocavity and the electrons bounce forth and back in the cavity thanks to the electron tunneling regime, controlling the intensity of the photons. (B) Energy level diagram where the two metallic walls of the cavity, separated by a distance S, are represented by their Fermi levels (EF), shifted when a DC external bias (U) is applied, producing a DC current (J_{dc}). The presence of the DC current modulates the optical current at frequency **ω** (J_{ω}), producing the electrooptical modulation effect at the nanoscale.

In Javier Aizpurua's words, researcher at CSIC-UPV/EHU joint Center for Materials Physics and DIPC:
"It is like using a very tiny room where we trap together electrons and photons, and the photons shine or quench depending on how the electrons bounce forth and back on the room's walls".

Controlling the activation or deactivation of the fast oscillations of light with static currents at this miniaturized level can be only possible due to the exquisite dependence of the trapped light to the tunneling regime of electrons across the nanogap. For the first time, the researchers propose a technological solution to create an electrooptical modulator at the nanoscale. The principle of action requires very precise fabrication of nanoscale gaps, where light can get trapped, as well as a convenient and simultaneous bias applied between these electrodes to control the DC tunneling current. Only under these conditions, electrooptical modulation at the nanoscale is possible.

The level of modulation can be optimized in future nanodevices, but this electrooptical concept at the nanoscale opens a door to the development of new technologies of information, where electrons and photons can talk faster and more packed, and thus with less consumption of energy per bit of information exchanged.

Electronic friction-based vibrational lifetimes of molecular adsorbates: Beyond the independent-atom approximation

S.P. Rittmeyer, J. Meyer, J.I. Juaristi, and K. Reuter
Physical Review Letters 115, 046102 (2015)

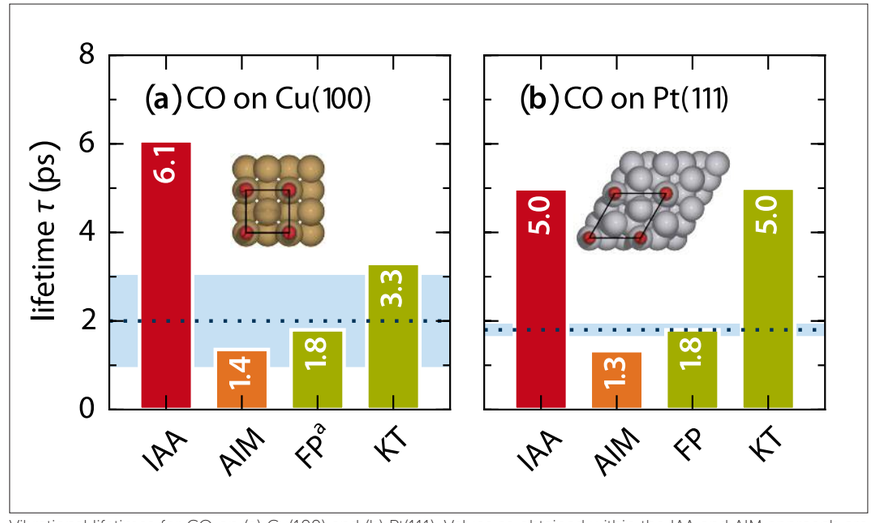
The damping of vibrational modes of molecules adsorbed on metal surfaces is usually governed by the energy transfer to electronic excitations. In this work, a new approach based on the electronic friction concept that goes beyond the independent atom approximation has been developed to treat this problem. The results show good agreement with available experimental data.

A very common approximation routinely relied on in molecular and condensed matter physics is the so-called adiabatic or Born-Oppenheimer approximation. Here one assumes that nuclear motion is much slower than the motion of the electrons such that the further can be assumed to remain in fixed positions. This approximation is very successful, but it is known to fail in certain cases.

For example, during chemical reactions on metal surfaces ions are moving through the metallic electron gas near the surface. Under these circumstances one could expect an electronic friction effect, which actually manifests as a stopping power that slows down the ions [1]. This electronic friction is thus a way of losing energy and can be attributed to electronic non-adiabaticity.

The study of these non-adiabatic ways of losing energy in surface reactions, especially catalytic reactions, is crucial in understanding also technological applications. But, to date, most accurate solutions of the full nuclear-electron wave function are restricted to systems of the complexity level of gas-phase H_2^+. For more complex systems further approximations have to be made, such as combined quantum and classical dynamics or perturbative approaches. Still, the imposed computational burden nevertheless restricts their practical use to simple metals and sub-picosecond time scales, to symmetric adsorbate trajectories, or to only qualitative accounts of the metal electronic structure.

An efficient way, in terms of computational demand, to do calculations with predictive quality and material specific trajectories would be to correct the Born-Oppenheimer approximation with classical molecular dynamics (MD) that incorporate the concept of electronic friction. Particularly, some recent attempts have been done using the local-density friction approximation (LDFA) and for molecular adsorbates an additional independent-atom approximation (IAA), that provides a further decrease in computational cost. However, due to the drastic simplifications introduced with the IAA, the validity of the LDFA formalism for molecular adsorbates per se has been controversially discussed.



Vibrational lifetimes for CO on (a) Cu(100) and (b) Pt(111). Values as obtained within the IAA and AIM approach are contrasted to corresponding predicted lifetimes published in the literature. For comparison, experimental values as obtained from pump-probe spectroscopy are shown as a dotted line and a blue stripe further indicating the reported experimental uncertainty.

Ions moving in metal electron gases lose energy due the electronic friction effect

In the present work, the researchers perform a substantiated assessment of the quality of the non-adiabatic description and propose a way to further improve it. In the study, accurate experimental reference data are used, primarily focusing on the vibrational damping of the internal stretch mode of two systems which have been studied most extensively and conclusively by experiments: CO adsorbed on Cu(100) and Pt(111). The authors find that rather than an explicit account of the surface band structure, missing intramolecular contributions within the independent atoms approximation are the reason for the main differences. Moreover, approximately incorporating such contributions through an atoms-in-molecules (AIM) embedding approach indeed yields consistent lifetimes for a range of diatomic adsorbate systems.

The presented AIM alternative accounts for energy dissipation approximately through a charge-partitioning scheme. As it effectively treats the molecular electrons as part of the metallic substrate, it is expected that the AIM friction concept to generally rather overestimate nonadiabatic energy losses and to perform best for chemisorbed adsorbates at close distances to the surface.

The results consolidate the trust in the concept of electronic friction and in particular the local-density friction approximation in the study of the technologically critical catalytic systems.

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Universal quantum transducers based on surface acoustic waves

M.J.A. Schuetz, E.M. Kessler, G. Giedke, L.M.K. Vandersypen, M.D. Lukin, and J.I. Cirac
Physical Review X 5, 031031 (2015)

"Quantum Computing" refers to the use of quantum effects to process information. In a "classical computer" information is held in bits, which can have two alternative values (0 and 1). In a "quantum computer" however, the unit of information is a quantum two-level system (qubit), which can be in any superposition of 0 and 1 or entangled with other qubits, enabling faster and more secure information processing.

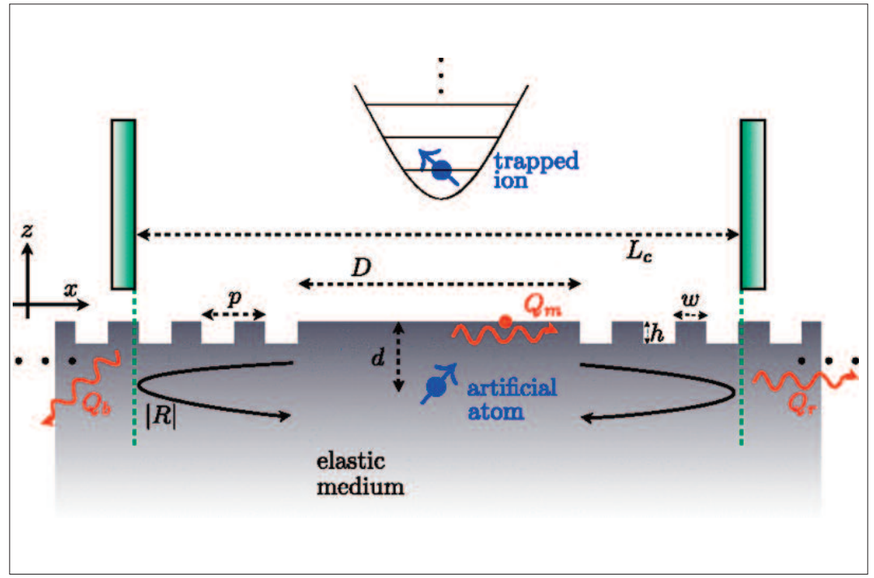
Qubits can be realized in solid-state based systems, e.g., by electron spins in quantum dots. A central challenge towards developing a scalable, solid-state spin-based quantum computer is to enable interaction between distant qubits. One approach to this goal is to couple the spins to mobile quantum systems (photons, phonons) that mediates the interaction. The transduction of quantum information between stationary and moving qubits is central to this approach. Now an international group of researchers that includes Geza Giedke, an Ikerbasque Research Professor working at DIPC, and led by Juan Ignacio Cirac, Director of the Max Planck Institute for Quantum Optics, propose a new quantum transducer and data bus based on surface acoustic waves (SAWs).

SAWs involve phonon-like excitations bound to the surface of a solid and are widely used in modern electronic devices. In piezoactive materials, SAWs are accompanied by electric or magnetic fields which facilitate coupling to different qubit realizations. The researchers analyze their coupling to SAW phonon resonator modes and show that the coherent qubit-resonator coupling dominates over noise processes, making available a slew of protocols for manipulating and coupling qubits.

This system has several appealing properties: it builds on established technology (SAW resonators and waveguides), it is not specific to any particular qubit, but provides a common platform for a range of qubit implementations (from trapped ions to quantum dots and superconducting circuits), and it uses an intrinsic degree of freedom – phonons – turning it from a liability (decoherence mechanism) into a valuable asset for coherent quantum control.

In summary, the researchers propose SAW phonons in piezoactive materials as a universal quantum transducer that allows to convert quantum information between stationary and propagating realizations. Using a combination of techniques from quantum optics and quantum information, this opens a way to on-chip acoustics-based quantum information processors.

Connecting qubits with sound



SAW as a universal quantum transducer. Distributed Bragg reflectors made of grooves form a resonator for SAWs. Reflection occurs effectively at some distance inside the grating.

This system provides a common platform for a range of qubit implementations

Direct observation of many-body charge density oscillations in a two-dimensional electron gas

P. Sessi, V.M. Silkin, I.A. Nechaev, T. Bathon, L. El-Kareh, E.V. Chulkov, P.M. Echenique and M. Bode
Nature Communications 6, 8691 (2015)

Interference is a general phenomenon that appears whenever we are dealing with the superposition of coherent waves. Because of the wave-particle duality, electrons can interfere. The invention of the scanning tunneling microscope (STM) allowed the visualization of this effect by looking at the spectacular standing wave patterns produced by elastic scattering of electrons and holes at surface defects: vacancies, adsorbates, impurities or step edges, to name a few.

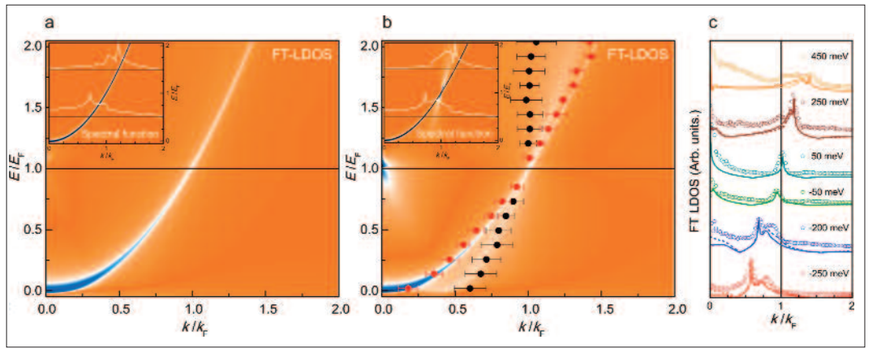
These waves, known as Friedel oscillations correspond to modulations of the electronic local density of states (LDOS). To date, quantum-interference measurements were mainly interpreted in terms of interfering electrons or holes of the underlying band-structure description.

In this work, by imaging energy-dependent standing-wave patterns at noble metal surfaces (the so-called quasi-particle interference (QPI) mapping), the researchers reveal, in addition to the conventional surface-state band, the existence of an 'anomalous' energy band with a well-defined dispersion. Its origin is explained by the presence of a satellite in the structure of the quasiparticle spectral function, which is related to a kind of surface plasmon, the so-called, acoustic surface plasmon. Visualizing the corresponding charge oscillations provides thus direct access to many-body interactions at the atomic scale. The results are published in Nature Communications.

Using STM measurements, the researchers were able to visualize how the Fermi sea locally rearranges to minimize the perturbation created by low-energy excitations. By analysing the QPI patterns produced around point defects at Cu, Ag and Au (111) surfaces, they found evidence that the two-dimensional electron gas of the surface of the metals exhibits an additional contribution to the electronic local density oscillations, which leads to extra modulations in the QPI and are related to the acoustic surface plasmon, a novel collective electronic excitation at metal surfaces that has a linear (or acoustic-like) dispersion.

The team also concludes that the secondary electrons and holes incoherently produced during the inelastic decay process of an injected quasi-particle can contribute to the formation of the QPI patterns as well. These secondary quasi-particles generate self-interfering patterns, which are cumulated to form the background contribution.

Plasmon: a collective excitation of electrons



(a,b) FT LDOS and underlying many-body spectral function (inset) for the conventional 2DEG and the 2DEG formed by surface-state electrons, respectively. The latter case is accompanied by the experimental data acquired for the Cu(111) surface. For comparison with the experimental data, we plot the FT LDOS as a function of k=p/2, where p is the magnitude of the reciprocal-space vector used in the formulas. In the insets, solid white lines show the spectral function as a function of the wavevector k at E=0.5EF and 1.5EF in logarithmic scale. (c) FT LDOS as a function of k=p/2 at a fixed energy E with (dashed lines) and without (solid lines) the background contribution in comparison with radially averaged line sections (open circles) as measured at different bias voltages for the Cu(111) surface. All the data are presented in relative units in order to underline the common nature of the considered phenomenon.

Many-body effects are usually challenging to be measured with spatial resolution

These findings expand the capabilities of the QPI mapping as an experimental technique to study many-body effects, which are relevant in several exciting areas of condensed matter physics, such as superconductivity and quantum information. Using a local probe to visualize many-body effects is expected to give important contributions to understanding unconventional physical properties on a microscopic scale.

Enhancement of near-field radiative heat transfer in polar dielectric thin films

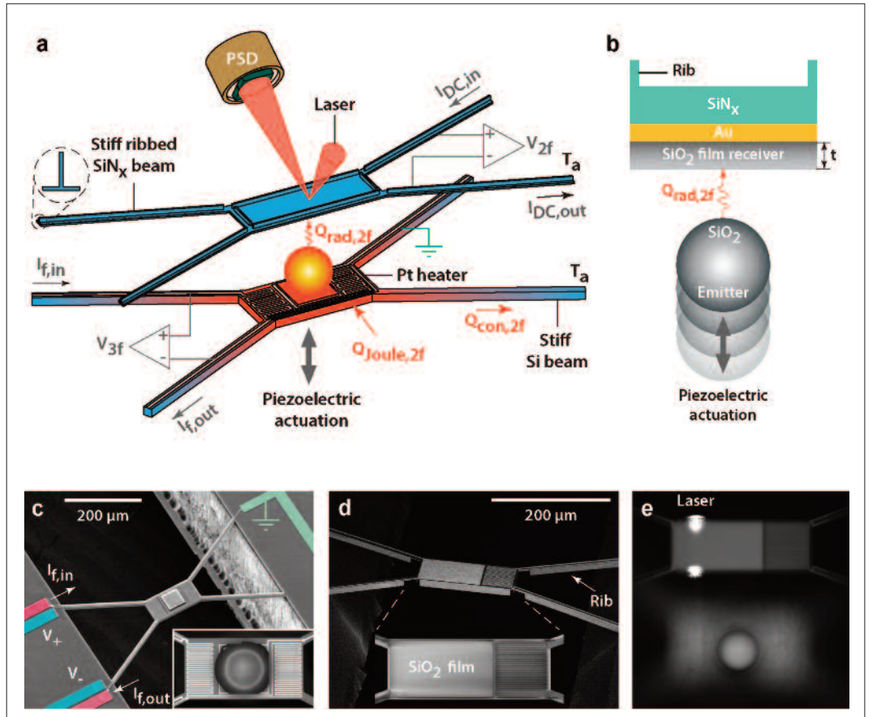
B. Song, Y. Ganjeh, S. Sadat, D. Thompson, A. Fiorino, V. Fernández-Hurtado, J. Feist, F.J. Garcia-Vidal, J.C. Cuevas, P. Reddy, E. Meyhofer
Nature Nanotechnology 10, 253 (2015)

Thermal radiation plays a major role in energy conversion, thermal management, and data storage. In recent years, several experiments on thermal radiation between bulk materials have demonstrated that radiative heat transfer can be greatly enhanced in nanoscale gaps.

However, it was not clear whether such enhancements could be obtained with nanoscale films thinner than the penetration depth of radiation. In this work, experimental researchers from the University of Michigan (the groups of Pramod Reddy and Edgar Meyhofer) have conducted near-field radiation experiments using a novel ultrasensitive calorimeter that demonstrate enhancements of several orders of magnitude in radiative heat transfer, even for ultra thin dielectric films (50 nm), at spatial separations comparable to or smaller than the film thickness.

A frequent visitor at DIPC (Francisco J. García-Vidal) along with his colleagues at IFIMAC (V. Fernández-Hurtado, J. Feist and JC. Cuevas) have explained these striking results making use of the theory of fluctuational electrodynamics. In particular, they have showed that the near field radiative heat transfer in polar dielectric thin films is determined by the excitation of cavity surface phonon polaritons. These surface electromagnetic modes have characteristic penetration depths that are of the order of the gap separating the receiver from the emitter.

In practice, this implies that the entire near field thermal radiation emitted by a polar material comes from its surface. Thus, the thermal emission of a polar thin film is independent of its thickness, as long as the gap between materials remains smaller than the film thickness. Our findings have important implications to a variety of future energy conversion and heat transfer nanotechnologies.



Experimental setup. **a**, Schematic of the experimental setup. The emitter consists of a suspended silicon platform, with an attached silica sphere, and an integrated electrical heater-thermometer. The receiver is a stiff silicon nitride platform coated with gold and a silica film of suitably chosen thickness. A laser (reflected off the receiver, see also e) and a position sensitive detector (PSD) enable emitter-receiver contact detection with nanometer resolution. **b**, Schematic cross section of the planar receiver region and the spherical silica emitter. The gold layer is ~100 nm thick, the thickness (t) of the SiO_2 film varies from 50 nm to 3 µm for different receiver devices. **c**, Scanning electron microscope (SEM) image of the suspended platform and optical image (inset) of the spherical emitter. **d**, SEM images of the receiver show ribbed beams and suspended regions. **e**, An optical image of the emitter and receiver during alignment. In this image the devices were laterally displaced to enable simultaneous visualization.

Comparing quasiparticle H_2O level alignment on anatase and rutile TiO_2

H. Sun, D.J. Mowbray, A. Migani, J. Zhao, H. Petek, A. Rubio
ACS Catalysis 5, 4242 (2015)

In heterogeneous catalysis, photocatalytic activity is controlled by the level alignment of the adsorbate and substrate levels. The position of the adsorbate's highest occupied molecular orbital (HOMO) levels relative to the substrate's valence band maximum (VBM) in the interface describes the favorability of photogenerated hole transfer from the VBM to the adsorbed molecule. For this reason it is essential to obtain a quantitative description of the interfacial level alignment to determine and predict catalytic activity. This can only be obtained from many-body quasiparticle *GW* calculations, which are necessary to correctly describe the anisotropic screening of electron-electron interactions at the catalysts interface, as depicted schematically in Figure 1.

We have performed an in-depth comparison of the G_0W_0 level alignment for water–anatase (H_2O–A-TiO_2(101)) and water–rutile (H_2O–R-TiO_2(110)) interfaces (*cf.* Figure 2) for a range of chemically significant structures in the limits of low and high H_2O coverage, intact to fully dissociated H_2O, and stoichiometric to O defective surface composition. Using their HOMO–VBM level alignment prior to irradiation $\varepsilon^{PDOS}_{HOMO} - \varepsilon_{VBM}$, we have established the following trends in their relative photocatalytic activity for H_2O photooxidation (*cf.* Figure 3). (1) There is a strong linear correlation between $\varepsilon^{PDOS}_{HOMO}$ on A-TiO_{2-x}(101) and R-TiO_{2-x}(110). (2) We consistently find H_2O's $\varepsilon^{PDOS}_{HOMO}$ closer to ε_{VBM} for A-TiO_2 than R-TiO_2. (3) These differences in $\varepsilon^{PDOS}_{HOMO}$ are greater for dissociated H_2O, and increase as $\varepsilon^{PDOS}_{HOMO}$ approaches ε_{VBM}. (4) Overall, $\varepsilon^{PDOS}_{HOMO}$ approaches ε_{VBM} with H_2O dissociation.

Altogether, this suggests HO@Ticus is more photocatalytically active than intact H_2O@Ticus and hole trapping is more favorable on A-TiO_2(101) than R-TiO_2(110). This may explain why the anatase polymorph is generally more photocatalytically active than rutile for H_2O photooxidation. Moreover, our results show how, in general, knowledge of an interfaces ground state electronic structure can be used to establish trends for predicting photocatalytic activity.

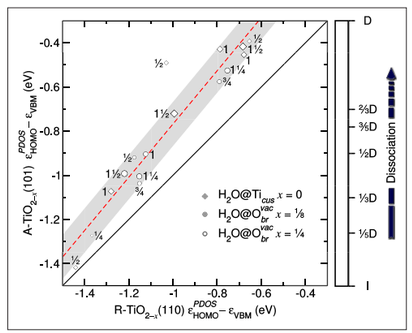


Figure 3: Average energy of water's G_0W_0 projected density of states highest occupied molecular orbital (HOMO) $\varepsilon^{PDOS}_{HOMO}$ relative to the surface's valence band maximum (VBM) ε_{VBM} in eV for H_2O adsorbed on coordinately unsaturated Ti sites (H_2O@Ti_{cus}) of stoichiometric anatase (A-TiO_2(101)) versus rutile (R-TiO_2(110)) and for H_2O adsorbed on bridging O vacancies (H_2O@O_{br}^{vac}) of defective anatase (A-TiO_{2-x}(101)) versus rutile (R-TiO_{2-x}(110)) for x = 1/8 or 1/4. H_2O total coverage in ML and fraction intact (I) or dissociated (D) are provided. A linear fit (red dashed line) with a standard deviation of ±0.1 eV (gray regions) is compared to the identity line (black solid line).

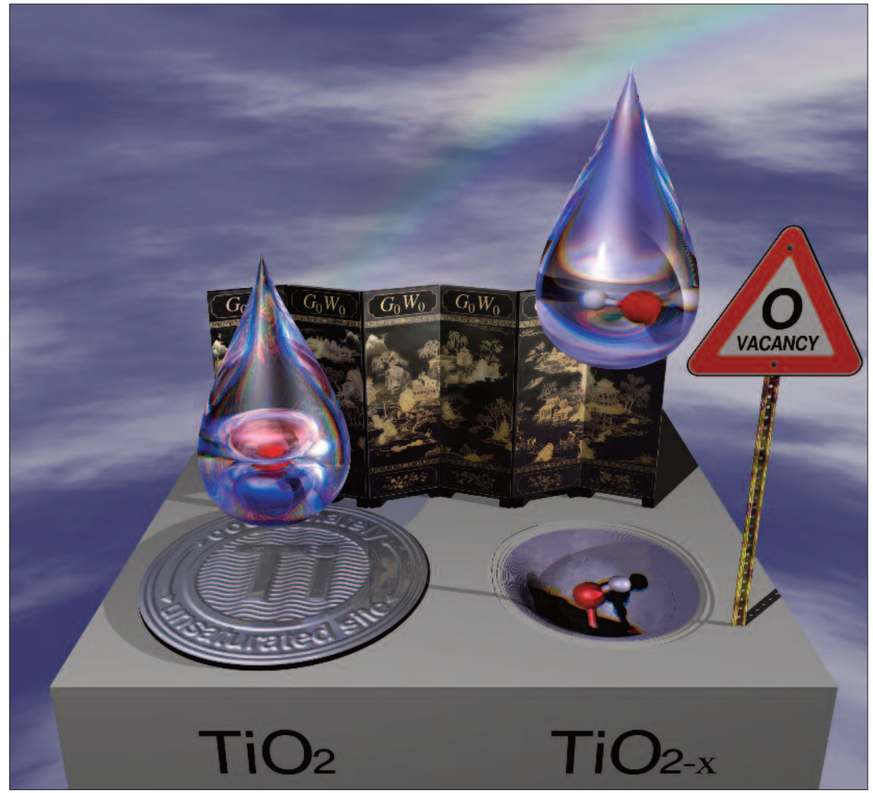


Figure 1: Electronic level alignment at molecule–surface interfaces controls the interface's photocatalytic activity. Many-body quasiparticle G_0W_0 theory is used to study the level alignment for water adsorbed intact and dissociatively on stoichiometric (left) and reduced (right) rutile and anatase titanium dioxide. This method includes the description of the anisotropic screening (screen) of the electron-electron interaction at molecule-surface interfaces, which is essential to obtain accurate interfacial level alignment for water's highest occupied molecular orbital (HOMO) $\varepsilon^{PDOS}_{HOMO}$ relative to the surface's valence band maximum (VBM) ε_{VBM}.

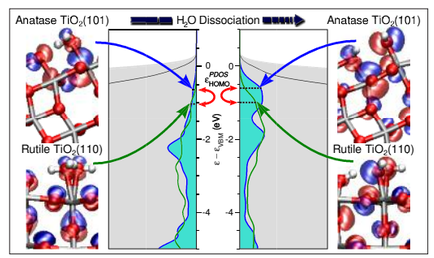


Figure 2: G_0W_0 total (grey/black) and H_2O projected (blue/green) density of states for 1ML intact (left) and 1/2 dissociated (right) H_2O adsorbed on coordinately unsaturated Ti sites (H_2O@Ticus) of anatase TiO_2(101)/rutile TiO_2(110) surfaces and water's highest occupied molecular orbital (HOMO) $\varepsilon^{PDOS}_{HOMO}$ relative to the surface's valence band maximum (VBM) ε_{VBM} in eV.

X-ray photoemission analysis of clean and carbon monoxide chemisorbed platinum(111) stepped surfaces using a curved crystal

A.L. Walter, F. Schiller, M. Corso, L.R. Merte, F. Bertram, J. Lobo-Checa, M. Shipilin, J. Gustafson, E. Lundgren, A.X. Brión-Ríos, P. Cabrera-Sanfelix, D. Sánchez-Portal and J.E. Ortega
Nature Communications 6, 8903 (2015)

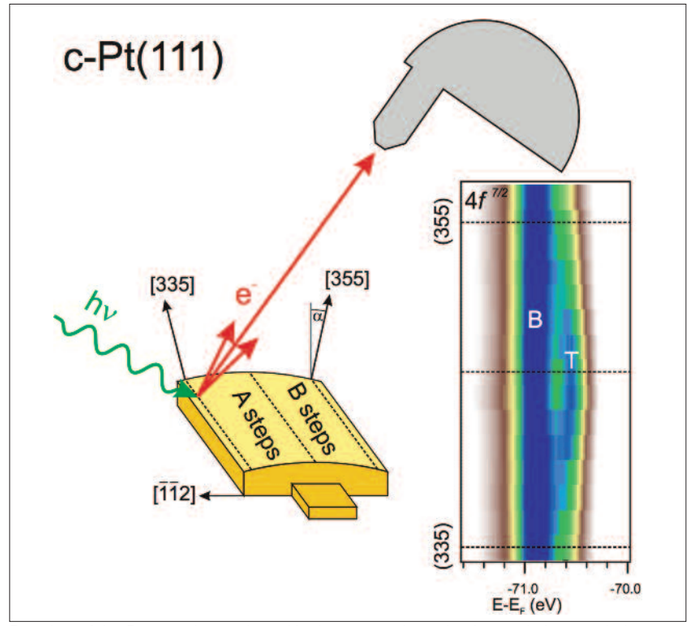
Surface steps are low atomic coordination sites and hence chemically and electronically very active. Stepped surfaces are thus frequently utilized to enhance or tune many physical-chemical processes, such as chemical reactions and epitaxial growth. However, it is not a-priori clear whether a stepped surface improves or worsens the growth of a specific material, or promotes or disturbs a given surface chemical reaction. One key parameter is the step density 1/d, which may be critical, for example, to enhance gas/surface heterogeneous catalysis. Using surfaces with curved shape one can smoothly vary the surface crystal orientation, that is, the step-density 1/d on a single sample, allowing a rational assessment of the influence of steps on physical-chemical processes.

Platinum is the benchmark of gas-solid chemistry studies. Over the past forty years dozens of works have been published about the fundamentals of chemical reactions and catalysis using platinum crystal surfaces as model platforms. Platinum (Pt) is at the basis of catalytic converters in the automobile industry. In fact, modern catalyzers feature nano-engineered oxide supports embedding active Pt nanoparticles, which speed up and optimize the CO-to-CO2 conversion. Researchers focus on single crystals to understand the CO oxidation process at a metal surface. They aim at identifying active atomic sites and tuning reaction kinetics, using the most powerful analytical technique for such studies: X-ray photoemission.

Why curving a Platinum crystal?
In the present study, published in Nature Communication, Walter et al. give a further push to fundamental research in the field of heterogeneous catalysis. They demonstrate that curved crystals can be readily utilized for high-resolution X-ray photoemission studies of CO chemisorption on stepped Pt(111), carried out at the synchrotron. By scanning the X-ray probe on the Pt curved surface, Walter et al. readily visualize the structure of atomic steps, the subtle relaxations in the Pt crystal lattice that steps allow, and, finally, the influence of all such properties in the simple CO chemisorption reaction.

The Pt curved crystals used in the study have been manufactured by Bihurcrystal, a company born in 2013 as a start-up project with support from the Material Physics Center (CSIC-UPV/EHU) and Donostia International Physics Center (DIPC).

The results offer the prospect of applying the curved surface approach to rationally investigate the chemical activity of surfaces under real pressure conditions



Drawing of the Pt curved crystal used in the present investigation and photoemission scan of the curved Pt(111) surface. XPS image showing the evolution of the Pt 4f spectra across the curved crystal. A characteristic step-density-dependent shift is observed in the surface component, revealing a 1/d-dependent release of tensile stress at the Pt surface.

Surface chemistry and catalysis studies could significantly gain from the systematic variation of surface active sites, tested under the very same conditions. Curved crystals are excellent platforms to perform such systematics, which may in turn allow one to better resolve fundamental properties and reveal new phenomena.

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Magnetic proximity effect in the layered structures.

Dr. Fabienne Barroso Bujans
Centro de Física de Materiales, CSIC-UPV/EHU, Donostia/San Sebastián, Spain
16/04/2013–14/09/2015
Aimed at finding the much-needed link between structure and properties of polymers confined at sub-nanometer dimensions at both fundamental and practical levels via understanding, tuning, and, ultimately, controlling the properties of polymer-based graphene nanostructured matter.

Dr. María de Gracia Retamosa Hernández
Facultad de Química, UPV/EHU, Donostia/San Sebastián, Spain
01/07/2013–Present
Remote structural effects in unnatural amino acids.

Dr. Mikhail Otrokov
State University of Tomsk, Russian Federation
17/07/2013–Present
Topological insulators.

Dr. Miren Iosune Arrastia Basalo
Facultad de Química, UPV/EHU, Donostia/San Sebastián, Spain
01/08/2013–Present
Multiple spin state reactivity in Fe-containing complexes and enzymes.

Dr. Elena Formoso Estensoro
Università della Svizzera Italiana, Lugano, Switzerland
01/02/2014–Present
Unveiling biochemical relevant structural conformations of the aluminum cation amyloid-beta peptide complex.

Dr. Federica Lo Verso
Material Physics Center, MPC, Donostia/San Sebastián, Spain
01/02/2014–Present
Structure and dynamics of complex materials based on polymers.

Dr. Luis Alejandro Miccio
UPV/EHU, Donostia/San Sebastián, Spain
17/07/2014–15/11/2015
Physical chemistry of curved surfaces.

Dr. Daniel Gosálbez Martínez
Centro de Física de Materiales and Universidad del País Vasco, Donostia/San Sebastián, Spain
15/09/2014–24/01/2015
Weyl nodes in ferromagnetic bandstructures.

Dr. Rémi Petuya
Institut des Sciences Moléculaires, Université Bordeaux, France
01/10/2014–Present
Characterization of structural and electronic properties of molecular overlayers on metal surfaces.

Dr. Jens Brede
Institute of Applied Physics and Interdisciplinary Nanoscience Center, Hamburg, Germany
27/10/2014–31/08/2015
Physical chemical reactions at surfaces: physico-chemical aspects.

Dr. Romain Dupuis
CEMES/CNRS, Toulouse, France
10/12/2014–Present
Cements and nanoadditions.

Dr. Ion Errea Lope
Institut de Minéralogie et de Physique de Milieux Condensés, Université Pierre et Marie Curie, Paris, France
01/01/2015–22/04/2015
Vibrational properties of bulk materials and nanostructures.

Dr. Eloy Ramos Cordoba
Universitat de Girona, Spain
01/01/2015–31/12/2015
Domain-averaged molecular Fermi holes and quantum molecular aromaticity.

Dr. Tatiana Novokhatskaya
Institute d'Electronique Fondamental, Orsay, France
01/01/2015–31/12/2015
Computational plasmonics.

Dr. Guillaume Vasseur
Institut Jean Lamour, Université de Lorraine-CNRS, France
05/01/2015–Present
Physics and chemistry of curved crystal surfaces.

Dr. Deung Jang Choi
Max Planck Institute, Hamburg, Germany
10/03/2015–30/04/2015
Spin dynamics of atomic objects on surfaces.

Dr. Joseba Alberdi Rodriguez
Facultad de Informática, UPV/EHU, Donostia/San Sebastián, Spain
01/07/2015–Present
Morfokinetics: development of computational techniques for the analysis of CVD growth of new 2D materials.

Dr. Marta Pelc
Nicolaus Copernicus University, Torun, Poland
01/12/2015–Present
Topological defects on carbon like nanostructures.

PhD Students

Alexander Correa Aristizabal
Universidad del Valle, Cali, Colombia
21/06/2011–20/06/2015
Studies at the nanoscale of interfaces for biosensor and solar cell applications.

Anton Xose Brion Rios
Universidad de Vigo, Spain
06/02/2013–Present
Theoretical study on the molecular adsorption and self-organization on substrates of different nature.

Dino Novko
University of Zagreb, Croatia
25/09/2013–Present
Non-adiabatic effects in the interaction of metal surfaces with atoms and small molecules.

Oihana Galparsoro Larraza
Facultad de Química, UPV/EHU, Donostia/San Sebastián, Spain
01/10/2013–Present
Phonon and electron excitations in diatom abstraction from metallic surfaces.

Bernhard Kretz
Gratz University of Technology, Gratz, Austria
09/06/2014–Present
Electronic and transport properties of graphenic nanostructures.

Tomas Neuman
Brno University of Technology, Czech Republic
01/09/2014–30/04/2015
Theory of scattering-type near-field microscopy and infrared spectroscopy.

Lucía Ortega Alvarez
Instituto de Ciencia y Tecnología de Polímeros/CSIC, Madrid, Spain
12/01/2015–Present
Structure and dynamics of silica filled rubber compounds.

Natalia Koval
Adygea State University, Russian Federation
21/01/2015–Present
Time-dependent density functional theory calculations of the energy loss of particles in metallic media.

Néstor Merino Diez
Universidad de la Rioja, Logroño, Spain
01/09/2015–Present
Functional materials synthesized by surface-supported chemistry under vacuum.

Visiting Researchers

Long visits

Dr. Rafael Grande Aztatzi
Cinvestav, Centro de Investigación y Estudios Avanzados del Instituto Politécnico Nacional, Mexico
28/08/2014–31/12/2016
Computational approach to aluminum biochemistry: al-phosphorylated polypeptide interactions.

Dr. Carlos Echeverria Arrondo
Facultad de Ciencia y Tecnología, UPV/EHU, Bilbao, Spain
15/09/2014–14/03/2015
Calculations on magnetic properties for ZnO nanoparticles.

Dr. Duncan Mowbray
Center for Atomicscale Materials Design, Technical University of Denmark, Lyngby, Denmark
01/01/2012–Present
Time-resolved oxyde mediated photocatalisis.

Dr. Hector Ochoa de Eguileor
Instituto Ciencia Materiales de Madrid, CSIC, Spain
03/11/2014–28/02/2015
Two-dimensional materials. Spin-orbit coupling (topology, spintronics).

Dr. Vitaly Golovach
CNRS Grenoble, France
01/11/2012–31/10/2017
Electronic properties at the nanoscale.

Mauricio Rodriguez Mayorga (PhD Student)
Universitat de Girona, Spain
01/12/2014–31/12/2017
Development of improved exchange-correlation functionals.

Dr. Mathias Ljunberg
Laboratoire ondes et matière d'Aquitaine (LOMA) - CNRS, Talence, France
16/04/2014–16/04/2016
First principles calculations of complex oxides.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, Mexico
15/12/2014–15/01/2015
Nanostructure materials.

Dr. Peng Zhang
Shanxi University, Taiyuan, China
18/08/2014–13/01/2015
Morphokinetics: Morphology-based modeling of the growth kinetics of 2D materials.

Prof. Istvan Nagy
Technical University of Budapest, Hungary
07/01–07/02/2015
Various aspects of correlations in extended fermionic systems; spin-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Prof. Matthew Dawber
Stony Brook University, New York, USA
07/01–27/02/2015
Ferroelectric oxides experimental condensed matter physics superlattices.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
10/01–28/02/2015
Surface phonons and phase transitions.

Laura Sánchez García (PhD Student)
Universidad Autónoma de Madrid, Spain
11/01–11/02/2015
Plasmonics assisting solid state lasing.

Andrea Basagni (PhD Student)
University of Padua, Italy
31/01–31/03/2015
Characterization of covalently bonded molecular chains synthesized by on-surface chemistry under ultra-high-vacuum.

Prof. Gernot Frenking
Fachbereich Chemie, Philipps Universität Marburg, Germany
01/02–30/04/2015
Theoretical chemistry.

Dr. Elizabeth Goiri Little
SUNY Korea (The State University of New York), Korea
02/02–30/06/2015
Donor acceptor monolayer blends on coinage metal surfaces.

Dr. Deung Jang Choi
Max Planck Institute, Hamburg, Germany
03/02–09/03/2015
Spin dynamics of atomic objects on surfaces.

Prof. Norman March
University of Antwerpen, Belgium
05/02–05/04/2015
Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

Dr. Arlette Violeta Richaud Torres
Universidad Autónoma Metropolitana, Iztapalapa, Mexico
13/02–31/12/2015
Development of new interpretative reactivity parameters derived from DFT and HSAB principle, based in chemical synthesis and molecular spectroscopic data.

Prof. Joseph R. Manson
Clemson University, Clemson, South Carolina, USA
19/02–30/03/2015
Theoretical studies of structure and dynamics of microscopic surfaces.

Prof. Roman O. Kuzian
National Academy of Sciences of Ukraine, Kiev, Ukraine
02/03–29/04/2015
Photoemission from strongly correlated systems.

Prof. Andrei Borisov
Université Paris Sud, France
06/04–30/06/2015
Quantum plasmonics

Prof. Alexander Protogenov
Institute of Applied Physics of Russian Academy of Sciences, Nizhnii Novgorod, Russian Federation
16/04–15/05/2015
Transport properties of 3D topological insulators.

Prof. Valery Tyuterev
Tomsk State Pedagogical University, Tomsk, Russian Federation
27/04–26/05/2015
Electron-phonon interaction and relaxation of highly excited carriers in wide-gap semiconductors.

Dr. Dana Codruta Marinica
Institut des Sciences Moléculaires d'Orsay, Université Paris Sud, France
01/05–30/06/2015
Quantum plasmonics.

Dr. Ziya Aliyev
Institute Catalysis and Inorganic Chemistry, Azerbaijan National Academy of Science, Azerbaijan
02/05–29/06/2015
Materials physics of topological insulators.

Prof. J. Alfredo Caro
Los Alamos National Laboratory, New Mexico, USA
02/05–30/06/2015
Theoretical simulation of radiation damage in nuclear materials.

Mario Zapata Herrera (PhD Student)
Universidad de Los Andes, Bogotá, Colombia
14/05–13/08/2015
Quantum effects in the plasmonic response.

Prof. Juan José Saenz Gutierrez
Universidad Autónoma de Madrid, Spain
17/05–31/07/2015
Light scattering in colloidal suspensions.

Prof. Ulrich Höfer
Philipps- Universität Marburg, Germany
01/06–31/07/2015
Resonance hopping on surfaces of simple metals.

Prof. Vladimir Menshov
National Research Centre "Kurchatov Institute", Moscow, Russian Federation
01/06–29/08/2015
Electron properties of magnetic topological insulator thin films.

Dr. Tatiana Menshchikova
Tomsk State University, Russian Federation
01/06–28/08/2015
Investigation of the electronic structure of topological insulators using first-principles calculations.

Dr. Igor Rusinov
Tomsk State University, Russian Federation
01/06–28/08/2015
Investigation of materials for spintronics: topological semiconductors and bismuth tellurohalides.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, Mexico
01/06–31/07/2015
Theoretical study of the electronic properties of transition metals on graphene sheet, and electronic properties of small binary clusters.

Prof. Carmen Mijangos Ugarte
Consejo Superior de Investigaciones Científicas Instituto de Ciencia y Tecnología de Polímeros Madrid, Spain
04/06–07/08/2015
Polymer structures with modulated morphologies and properties at nanoscale.

Dr. Sergey Eremeev
Institute of Strength Physics and Materials Science, Tomsk, Russian Federation
16/06–12/09/2015
Topological insulators.

Dr. José Surga Diaz
Petroleos de Venezuela S.A. PDVSA-INTEVEP Venezuela
17/06–15/09/2015
Cements under presure and temperature.

Prof. Vasily Astratov
University of North Carolina at Charlotte, USA
18/06–18/07/2015
Microspherical Photonics

Prof. Antonio Politano
Università degli Studi della Calabria, Italy
20/06–19/07/2015
Plasmon modes in topological insulators: from basic research to applications in plasma-wave THz photodetection.

Dr. Angela Demetriadou
Imperial College London, United Kingdom
21/06–19/09/2015
Nanophotonics in ultranarrow gaps.

Prof. Francisco Javier Muñoz Saez
Universidad de Chile, Ñuñoa, Santiago, Chile
29/06–02/08/2015
Topological insulators.

Prof. Nikolay Kabachnik
Institut fur Experimentalphysik, Hamburg, Germany
01/07–30/09/2015
Study of Auger processes in gases and at solid surfaces within an attosecond streaking scheme.

Prof. Francisco Guinea López
Inst.Ciencia Materiales de Madrid.CSIC, Madrid, Spain
01/07–31/07/2015
Condensed matter physics.

Prof. Francisco José García Vidal
Facultad de Ciencias, Universidad Autónoma de Madrid, Spain
01/07–31/08/2015
Plasmonics

Prof. Peter Bauer
Johannes Kepler University Linz
Institute of Experimental Physics, Austria
01/07–01/08/2015
Electronic stopping of slow ions

Prof. Luis Martín Moreno
Instituto de Ciencia de Materiales de Aragón, (ICMA), Zaragoza, Spain
01/07–31/07/2015
Optical properties of nanoscale systems.

Prof. Maria Angeles Hernández Vozmediano
Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, CSIC, Madrid, Spain
01/07–31/07/2015
Analysis of interactions, disorder, and lattice distortions in topological insulators and graphene.

Anastasiia G. Ryabishchenkova (PhD Student)
Tomsk State University, Russian Federation
01/07–15/08/2015
Atomic properties of topological insulators.

Dr. Igor V. Silkin
Tomsk State University, Tomsk, Russian Federation
01/07–01/08/2015
Topological insulators.

Prof. Miguel Angel Cazalilla
National Tsing Hua University, Taiwan
12/07–12/09/2015
Strongly correlated systems, 2D materials, spintronics.

Prof. Teunis Klapwijk
University of Delft, Holland
20/07–21/08/2015
Superconducting hybrid structures.

Prof. Vladimir M. Kuznetsov
Tomsk State University, Tomsk, Russian Federation
31/07–30/08/2015
Topological insulators.

Prof. Wlodzimierz Jaskólski
Institute of Physics Nicolaus Copernicus University, Poland
16/08–30/09/2015
Defects, edge states and magnetic effects in graphene structures.

María Ëugenia Sandoval Salinas
Universidad Nacional Autónoma de México, Mexico
24/08–17/11/2015
Singlet fission model in the FMO complex.

Grabiele Dalla Torre
Universita degli Studi di Milano, Italy
01/09–01/12/2018
Theoretical Chemistry

Prof. Marijan Sunjic
University of Zagreb, Croatia
02/09–29/10/2015
Dynamical response and surface excitations in thin films.

Prof. Amand Lucas
University of Namur, Belgium
03/09–30/10/2015
Surface science, ion scattering.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
09/09–31/10/2015
Surface phonons and phase transitions.

Prof. Joseph R. Manson
Clemson University, Clemson, South Carolina, USA
24/09–10/11/2015
Theoretical studies of structure and dynamics of microscopic surfaces.

Prof. Pedro De Andrés
Instituto Ciencia de Materiales de Madrid, CSIC, Madrid, Spain
01/10–27/11/2015
Life time of image states in graphene.

Dr. Ziya Aliyev
Institute Catalysis and Inorganic Chemistry, Azerbaijan National Academy of Science, Azerbaijan
01/10–29/12/2015
Materials physics of topological insulators.

Víctor Ramón Escobedo Bermúdez (PhD Student)
Universidad de Salamanca, Spain
01/10/2015–30/09/2016
Literature and Science.

Yuan Li (PhD Student)
Southeast University, Nanjing, China
04/10–22/12/2015
Reaction mechanism and diffusion model for the simulation of focused ion beam etching.

Flávio Matias da Silva (PhD Student)
Universidade General do Rio Grande do Sul, Porto Alegre, Brazil
15/10/2015–14/10/2016
Electronic excitations in metallic media using time-dependent density functional theory.

Prof. Julio A. Alonso Martín
Facultad de Ciencias, Universidad de Valladolid, Spain
25/10–25/11/2015
Adsorption and diffusion of hydrogen on nanoparticles.

Jon Lafuente Bartolomé (PhD Student)
Facultad de Ciencia y Tecnología, UPV/EHU, Leioa, Spain
01/11–31/12/2015
Relativistic corrections to response functions in 2D systems.

Prof. Raffaele Resta
Università di Trieste, Italy
01/12/2015–29/02/2016
Geometry and topology in electronic structure.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, Mexico
10/12/2015–10/01/2016
Theoretical study of the electronic properties of transition metals on graphene sheet, and electronic properties of small binary clusters.

Natalia Cortés Muñoz
Universidad Técnica Federico Santamaria, Valparaiso, Chile
16/12/2015–15/06/2016
Electronic and thermal properties of two dimensional materials.

Short visits

Prof. Rosa Bulo
University of Utrecht, Netherlands
11/01–16/01/2015
Hamiltonian adaptive QM/MM: multi-scale modeling of chemical reactions in solution.

Dr. Joachim Kohlbrecher
Paul Scherrer Institut, Villigen, Switzerland
12/01–14/01/2015
Magnetic response of functionalized lipid bilayers.

Prof. Godfrey Gumbs
Hunter College, The City University of New York, USA
05/01–30/01/2015
Plasmons in nanostructures.

Prof. Marivi Fernandez-Serra
Stony Brook University, New York, USA
07/01–21/01/2015
Condensed matter theory, first-principles simulations of condensed matter. First-principles simulation of liquid water and the interface between liquid water and solids quite generally, and applied to energy purposes (water photolysis etc).

Dr. Lucian Constantin
Italian Institute of Technology, Lecce, Italy
11/01–22/01/2015
Density Functional Theory

Prof. Larry Glasser
Clarkson University, USA
11/01–17/01/2015
Mathematical physics applied to condensed matter.

Prof. Jeffry A. Kelber
University of North Texas, Denton, USA
14/01–16/01/2015
Direct growth of 2D materials on practical substrates: from surface chemistry to new physics and devices.

Prof. Juan Ignacio Cirac
Max-Planck-Institut für Quantenoptik, Garching, Germany
15/01–16/01/2015
Quantum physics and computation.

Dr. Juan Pablo Echeverry Enciso
Humbolt University, Berlin, Germany
25/01–31/01/2015
Low-energy collective electronic excitations in graphite intercalated compounds.

Prof. Dieter Richter
IFF-FZ, Forschungszentrum Jülich, Germany
26/01–28/01/2015
Polymer dynamics by neutron techniques.

Prof. Pilar Goya Laza
Instituto de Química Médica (CSIC), Madrid
28/01–29/01/2015
Iatrochemistry, cannabis and drug design.

Prof. Juan José Gómez-Cadenas
Instituto de Fisica Corpuscular CSIC-UV, Valencia
29/01–30/01/2015
Landscape without neutrinos.

Prof. Marijan Sunjic
University of Zagreb, Croatia
02/02–27/02/2015
Dynamical response and surface excitations in thin films.

Prof. Arturo Tagliacozzo
Università di Napoli Federico II, Napoli, Italy
08/02–13/02/2015
Superconductivity.

Martin Schütz (PhD Student)
MPQ Garching, Germany
09/02–14/02/2015
Surface acoustic waves as a universal platform for quantum information processing.

Dr. Geza Toth
Ikerbasque, Dep. Theoretical Physics, UPV/EHU, Leioa, Spain
10/02–10/02/2015
Detection of multipartite entanglement close to symmetric Dicke states.

Prof. Angel J. Marzocca
Fate y Universidad de Buenos Aires, Argentina
15/02–16/02/2015
Rubber composites.

Prof. Jonas Fransson
Uppsala University, Sweden
15/02–16/02/2015
Electrical and thermal control of magnetic exchange interactions.

Prof. Carl Mitcham
Colorado School of Mines, USA
16/02–17/02/2015
Contributions of Physics to Ethics:
Nuclear Weapons, Free Will, and the Good Life

Prof. Salvador Miret Artes
CSIC, Madrid
22/02–25/02/2015
Theory of surface diffusion.

Prof. Ulrich Heinzmann
University of Bielefeld, Molecular & Surface Physics Bielefeld Institute for BioPhysics & NanoScience (BINAS) , Germany
23/02–27/02/2015
Atophysics.

Dr. Andrey Vasenko
Laboratoire de Physique et Modelisation des Milieux Condensed, CNRS, Grenoble, France
23/02–27/02/2015
Topological Insulator-Superconductor hybrid junctions.

Dr. Andrea Trabattoni
Politecnico di Milano, Italy
24/02–26/02/2015
Attosecond electron dynamics in complex molecular systems.

Dr. Amadeo Lopez Vazquez de Parga
Universidad Autónoma de Madrid, Spain
25/02–26/02/2015
Graphene growth and spectroscopy with low-T STM.

Prof. Dimitri Batani
Université de Bordeaux, Talence, France
25/02–26/02/2015
Development of the PETAL laser facility and its applications in physics

Prof. Vladimir Nazarov
Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan
26/02–25/03/2015
Time-dependent density-functional theory of EELS of thin films on substrates.

Prof. Michel Mortier
ParisTech, Ecole Nationale Superieure de Chimie de Paris, France
26/02–28/02/2015
Rare earth doped fluoride materials for optics and photonics.

Prof. Andreas Savin
Université Pierre et Marie Curie, Paris, France
UPMC Sorbonne Universités
Laboratoire de Chimie Théorique
02/03–13/03/2015
Adiabatic connection in DFT

Dr. Isabel Guillamon Gomez
Instituto de Ciencia de Materiales Nicolás Cabrera, Condensed Matter Physics Center, Universidad Autónoma de Madrid, Spain
05/03–06/03/2015
Scanning tunneling spectroscopy of the superconducting vortex lattice.

Prof. Antti-Pekka Jauho
Center for Nanostructured Graphene (CNG), DTU Nanotech, Technical University of Denmark
08/03–10/03/2015
Theoretical nanotechnology, nanostructured graphene, quantum transport.

Prof. Geert-Jan Kroes
Leiden Institute of Chemistry, Gorlaeus Laboratory, Leiden, The Netherlands
08/03–10/03/2015
Reactions of molecules at surfaces: dynamics and non-adiabatic effects, applications to hydrogen storage, astrochemistry.

Prof. Jean Marie Lehn
Université de Strasbourg, France
09/03–12/03/2015
Supramolecular chemistry.

Prof. Garnett Bryant
NIST, Gaithersburg, Maryland, USA
14/03–22/03/2015
Nanophotonics.

Dr. Hyowon Kim
Samsung Advanced Institute of Technology (SAIT)
Yeoungtong-gu, Suwon-si, Korea
14/03–17/03/2015
STM in graphene.

Dr. Sananda Biswas
International Centre for Theoretical Physica (ICTP), Trieste, Italy
15/03–22/03/2015
Anharmonic effects in lithium hydride.

Dr. Ana Montserrat Rosell
TVE programa Tres14, Madrid, Spain
17/03–18/03/2015
Science outreach.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, Mexico
22/03–27/03/2015
Theoretical study of the electronic properties of transition metals on graphene sheet, and electronic properties of small binary clusters.

Prof. Gines Morata
Centro Biología Molecular, Universidad Autónoma Madrid, Spain
23/03–24/03/2015
The fruit fly Drosophila to investigate the genetic basis of Cancer.

Dr. Jean-Christophe Gimel
Micro and Nano-medicine Laboratory, University Hospital in Angers, France
24/03–26/03/2015
Step polymerization in various solvent conditions. A computer simulation approach using "Patchy Brownian Cluster Dynamics".

Dr. Rémi Avriller
CNRS Laboratoire Ondes et Matière d'Aquitaine (LOMA) Université de Bordeaux et CNRS, Talence, France
25/03–27/03/2015
Quantum transport and nanoelectromechanical systems.

Prof. Yuliy Bludov
Center for Physics, University of Minho, Braga, Portugal
25/03–28/03/2015
Linear and nonlinear graphene plasmonics.

Dr. Bruce Milne
Centre for Computational Physics, University of Coimbra, Portugal
12/04–18/04/2015
Theoretical spectroscopy of the light harvesting complex from green plants.

Prof. Javier García de Abajo
ICFO - The Institute of Photonic Sciences, Castelldefels, Barcelona, Spain
13/04–15/04/2015
Nanoplasmonics at the single atomic layer level.

Prof. Helen Jansson
Chalmers University, Sweden
15/04–19/04/2015
Water dynamics under hard confinements.

Dr. Raffaello Bianco
Paris VI (UPMC), París
16/04–15/05/2015
Determination of the the charge-density phase transition temperature in $TiSe_2$ from the stochastic self-consistent harmonic approximation.

Prof. Anatoli Kheifets
Australian National University, Canberra (Australia)
23/04–29/04/2015
Strong field atomic ionization with light: spectra, cusps and time delay.

Prof. Denis Vyalikh
Dresden University of Technology, Dresden, Germany
26/04–30/04/2015
Photoemission measurements of magnetic surface states.

Dr. Angela Demetriadou
Imperial College London, United Kingdom
27/04–29/04/2015
Nanophotonics in ultranarrow gaps.

Dr. Marta Macho Stadler
Universidad del País Vasco (UPV/EHU), Lejona, Spain
28/04–29/04/2015
A través del espejo: la literatura mira a las científicas.

Eduardo Granados (PhD Student)
SLAC National Accelerator Laboratory, Stanford University, California, USA
29/04–30/04/2015
Exploring matter under extremes conditions at the linac coherent light source.

Prof. Manuel Toharia Cortés
Ciudad de las Artes y las Ciencias de Valencia, Spain
13/05–14/05/2015
La imperfección de los modelos del clima.

Prof. Luis Rosales Ahumada
Universidad Técnica Federico Santa María, Chile
17/05–23/05/2015
Bound states in the continuum in graphene based nanostructure.

Prof. Ranko Richert
Arizona State University, Tempe, USA
18/05–21/05/2015
Basics and applications of nonlinear dielectric techniques.

Prof. Pilar Hernández Gamazo
Instituto de Física Corpuscular CSIC-UV, Valencia, Spain
21/05–22/05/2015
Outlook in neutrino physics.

Prof. Francesc Monrabal Capilla
Texas A&M University (USA).
21/05–22/05/2015
Double beta decay in neutrino physics.

Prof. Juan José Gómez-Cadenas
Instituto de Fisica Corpuscular CSIC-UV, Valencia, Spain
21/05–22/05/2015
Landscape without neutrinos.

Lucie Stolcová (PhD Student)
Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Czech Republic
24/05–19/06/2015
Electrodynamic simulations for SERS-active substrates.

Dr. Omjyoti Dutta
Jagiellonian University, Krakow, Poland
27/05–30/05/2015
Quantum simulation and artificial matter with ultracold atoms, molecules, and quantum optics.

Dr. Gilles Buchs
Swiss Center for Electronics and Microtechnology, CSEM, Switzerland
31/05–06/06/2015
Engineering of the electronic and opto-electronic properties of carbon nanotubes via artificially induced defects and electrostatic doping.

Dr. Martin Schäffer
Technische Universität München, Germany
31/05–04/06/2015
Attosecond spectroscopy on surfaces.

Dr. Gervasi Herranz Casabona
Instituto de Ciencia de Materiales de Barcelona, Spain
01/06–03/06/2015
Magnetooptics.

Dr. Jonathan Rodriguez Fernandez
IMDEA, Madrid, Spain
04/06–05/06/2015
Charge transfer between donor-acceptor molecular networks on metal surfaces.

Prof. Luisa Bausa
Universidad Autónoma de Madrid, Spain
10/06–11/06/2015
Solid state laser assisted by plasmonics.

Laura Sánchez García (PhD Student)
Universidad Autónoma de Madrid, Spain
10/06–11/06/2015
Solid state laser assisted by plasmonics.

Prof. Giorgio Benedek
Universitá degli Studi di Milano-Bicoca, Milano, Italy
16/06–27/06/2015
Surface phonons and phase transitions.

Dr. Nuno De Sousa
Universidad Autónoma de Madrid, Spain
17/06–26/06/2015
Magneto-optics in random media.

Dr. Shigeki Kawai
University of Basel Switzerland PRESTO and Japan Science and Technology Agency, Kawaguchi, Japan
17/06–19/06/2015
Chemical Structures and mechanical propertis of molecules studied by high-resolution foce microscopy.

Dr. Elsa Perrin
Laboratoire de Chimie, Pasteur,
Ecole Normale Superieure de Paris, France
22/06–27/06/2015
Electronic structure of molecular solids.

Prof. Arturo Tagliacozzo
Università di Napoli Federico II, Napoli, Italy
22/06–25/06/2015
Superconductivity.

Prof. Dieter Richter
IFF-FZ, Forschungszentrum Jülich, Germany
22/06–25/06/2015
Polymer dynamics by neutron techniques.

Dr. Ivan Infante
Vrije Universiteit Amsterdam, Netherlands
23/06–26/06/2015
Modelling colloidal semiconductor nanocrystals: towards realistic sizes.

Prof. María Chamarro Calvo
Pierre and Marie Curie University,
Institut des NanoSciences de Paris, France
24/06–25/06/2015
Optical properties of semiconductors nanostructure.

Dr. Vladimir N. Strokov
Swiss Light Source and Paul Scherrer Institute,
Villigen-PSI, Switzerland
25/06–28/06/2015
Soft x-ray angle-resolved photoemission.

Prof. Ralf Tonner
Philipps-Universität Marburg, Germany
25/06–27/06/2015
First-principles simulations of organic-inorganic interfaces.

Prof. Robert Berger
Philipps-Universität Marburg, Germany
25/06–27/06/2015
First-principles simulations of organic-inorganic interfaces.

Prof. Vladimir Chaldyshev
Ioffe Physico Technical Institute, St.Petersburg, Russian Federation
27/06–04/07/2015
Plasmonics in GaAs-based materials.

Prof. Moty Heiblum
Weizmann Institute of Science, Rehovot, Israel
01/07–03/07/2015
Quantum Hall physics and topological superconductivity.

Prof. Antonios Balassis
Fordham University, New York, USA
01/07–29/07/2015
Collective excitations and Kohn anomaly in graphene.

Dr. Xiao Hu
International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), Tsukuba, Japan
05/07–08/07/2015
Simple design of topological state.

Prof. Didier Lemoine
Université Paul Sabatier, IRSAMC - LCAR, France
11/07–14/07/2015
Quantum and quasi-classical molecular dynamics simulations of molecule recombination processes at the gas-surface interface.

Prof. Bret Jackson
University of Massachusetts Amherst, USA
11/07–14/07/2015
Quantum and quasi-classical molecular dynamics simulations of molecule recombination processes at the gas-surface interface

Prof. Denis Vyalikh
Dresden University of Technology, Dresden, Germany
11/07–16/07/2015
Photoemission measurements of magnetic surface ststes.

Dr. Jerzy Cioslowski
University of Szczecin, Poland
11/07–26/07/2015
Density matrix functional theory and the harmonium atom.

Prof. Giorgio Benedek
Universitá degli Studi di Milano-Bicoca, Milano, Italy
14/07–18/07/2015
Surface phonons and phase transitions.

Prof. Chris Rossel
President of the European Physical Society
15/07–17/07/2015
Institutional visit.

Dr. Andrey Vasenko
Laboratoire de Physique et Modelisation des Milieux Condensed, CNRS, Université Joseph Fourier, Grenoble, France
16/07–15/08/2015
Properties of topological insulator superconductor interfaces.

Dr. Xavier Cartoixà Soler
Universidad Autónoma de Barcelona, Spain
23/07–25/07/2015
Transport in graphene-based devices.

Richard Berndt (PhD Student)
University of Kiel, STM, Germany
29/07–05/08/2015
STM-based spectroscopies of single-molecule and single-atom contacts.

Dr. Pablo Burset Atienza
University of Würzburg, Germany
03/08–08/08/2015
Josephson effect in Topological Insulators and Graphene.

Prof. Andrew F. Ho
Royal Holloway University College,
University of London, United Kingdom
17/08–22/08/2015
Low dimensional systems.

Prof. Barbara Kraus
Institut für Theoretischen Physik,
Universät Innsbruck, Austria
01/09–05/09/2015
Entanglement and entanglement transformations in fermionic systems.

Cornelia Spee (PhD Student)
Institut für Theoretischen Physik,
Universität Innsbruck, Austria
01/09–05/09/2015
Entanglement and entanglement transformations in fermionic systems.

Prof. Archie Howie
Cavendish Laboratory, Cambridge, United Kingdom
03/09–17/09/2015
Theory of valence electron excitations by fast electrons.

Prof. Wanda Andreoni
Ecole Polytechnique Federale de Lausanne,
EPFL Institute of Theoretical Physics, Switzerland
05/09–29/09/2015
Ab initio simulations of aqueous solutions for CO_2 capture and of nanostructures.

Dr. Juan Pablo Echeverry Enciso
Humbolt University, Berlin, Germany
06/09–10/09/2015
Low-energy collective electronic excitations in graphite intercalated compounds.

Dr. Leonor Chico Gómez
Instituto de Ciencia de Materiales de Madrid (ICMM), Spain
09/09–18/09/2015
Electronic structure calculations in nanotubes.

Prof. Pere Alemany Cahner
Universidad de Barcelona, Spain
10/09–11/09/2015
Electronic structure and symmetry.

Prof. Emi Minamitani
Graduate School of Engineering,
The University of Tokyo, Bunkyo-ku, Japan
11/09–26/09/2015
Theoretical studies on surface magnetism and surface phonons.

Prof. Andres Felipe Santander Syro
CSNSM, Université Paris-Sud, France
16/09–20/09/2015
Novel 2D electron gases at the surface of transition-metal oxides.

Prof. Salvador Miret Artes
CSIC, Instituto de Física Fundamental, Madrid, Spain
27/09–01/10/2015
Theory of surface diffusion.

Prof. Kurt Binder
Johannes Gutenberg University, Mainz, Germany
29/09–01/10/2015
Understanding the stiffness of Macromolecules: From single chains to semi flexible polymer brushes.

Dr. Enrique Rico Ortega
UPV/EHU Facultad Físico Química, Leioa, Spain
03/10–03/11/2015
Quantum simulators of gauge models.

Prof. José Ignacio Fernandez Vera
FECYT, Madrid, Spain
06/10–06/10/2015
FECYT and its role in science communications.

Prof. Holger Meyerheim
Max Planck Institute, Halle, Germany
07/10–10/10/2015
Structural investigations of topological insulators.

Prof. Remi Carminatti
Institut Langevin, ESPCI ParisTech, France
11/10–17/10/2015
Statistics of single molecule fluorescence lifetimes in random media.

Prof. John Schotland
University of Michigan, USA
11/10–17/10/2015
Optics of complex media.

Luciano Colazzo (PhD Student)
Universita de Padua, Italy
12/10–26/10/2015
Surface supported polymerization studies under ultra-high vacuum.

Prof. Bo Hellsing
Chalmers and Göteborg University, Sweden
13/10–22/10/2015
Electron-phonon interactions on metal surfaces.

Prof. Andrei Borisov
Université Paris Sud, France
18/10–24/10/2015
Quantum plasmonics

Prof. David Jeffery Wineland
NIST, Boulder, Colorado, USA
18/10–24/10/2015
Atomic ions confinement in electromagnetic traps.

Dr. Luis Froufe Perez
University of Fribourg, Switzerland
20/10–23/10/2015
Soft matter and photonics.

Dr. Nicolas Bonod
CNRS, Institute Fresnel, Marseille, France
22/10–27/10/2015
Resonant photonics, electromagnetism, nanophotonics.

Dr. Ignacio Arganda Carreras
University ofthe Basque Country, UPV/EHU, Spain
29/10–29/10/2015
Image processing tools for the study of brain connections.

Prof. John Inglesfield
University of Wales Cardiff, United Kingdom
04/11–28/11/2015
Study of the properties of resonance states, using embedding and their application to surface resonances.

Dr. Omjyoti Dutta
Jagiellonian University, Krakow, Poland
05/11–07/11/2015
Quantum simulation and artificial matter with ultracold atoms, molecules, and quantum optics.

Luca Salassa (PhD Student)
CIC BiomaGUNE, San Sebastián, Spain
06/11–06/11/2015
Hybrid upconversion nanomaterials for photochemotherapy.

Rodrigo Leiva (PhD Student)
Instituto de Astrofísica, Facultad de Física, Pontificia Universidad Católica de Chile and
Observatoire de Paris, LESIA, France
11/11–11/11/2015
Stellar occultations: Chariklo and its ring system.

Prof. Yousoo Kim
Surface and Interface Science Laboratory Riken,
Wako-shi, Saitama, Japan
12/11–14/11/2015
Atomic and molecular manipulation with the STM.

Dr. Marta Pelc
CFM, Centro de Física de Materiales, San Sebastián, Spain
19/11–19/11/2015
Topological defects on carbon like nanostructures.

Dr. Grigori Tkachov
Würzburg Universität, Germany
10/12–12/12/2015
T Signatures of the triplet superconductivity in topological insulator/ferromagnet contacts.

Dr. Pawel Rejmak
Institute of Physics, Polish Academy of Science, Warsazawa, Poland
14/12–15/12/2015
First-principles calculations on nanostructures.

Prof. Alberto Galindo Teixeira
Universidad Complutense de Madrid, Spain
14/12–15/12/2015
Quantum information and quantum algorithms. Basic problems in quantum physics.

Ikerbasque Research Professors

Prof. Vyacheslav Silkin
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. Eugene Krasovskii
Electronic structure of nanosystems, surfaces and interfaces. Attosecond time resolved photo-electron spectroscopy to study the dynamics of electronic excitations. Development of new computational methods of the density funtional theory.

Prof. Andrey Kazanskiy
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. Slawomir Grabowski
Hydrogen bonds in gas phase and crystals; quantum theory of atoms in molecules and natural bond orbitals approaches; intermolecular interactions as preliminary stages of chemical reactions.

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

Prof. Mario Piris Silveira
Energy functional method development. Computational modelling of semiconductor nanocluster and molecular solid phases and polymorfism.

Prof. Thomas Frederiksen
Quantum transport theory and electronic structure methods.

Prof. Geza Giedke
Quantum information and quantum optics: implementations of QIP in atomic and solid-state systems.

Prof. Davide Donadio
Theory of nanostructures and transport.

Prof. Dimas Garcia de Oteyza
Physical chemistry phenomena in organic materials and organic-inorganic interfaces.

Prof. Juan José Saenz Gutierrez
Nanophotonics. Modeling scanning probe microscopies.

Ikerbasque Research Fellows

Dr. Arantzazu Garcia Lekue
Modeling electron transport at the nanoscale. Theoretical investigation of electron processes at nano-structured surface.

Dr. María José Cabrera San Félix
Molecular level understanding of the interaction of molecules (particularly water) with surfaces and their self-assembly to form extended structures. Electronic and structural properties of clean and decorated surfaces: surface reconstructions and chemical reactivity.

Dr. Dario Bercioux
Quantum transport in defected carbon-nanotubes.

Dr. Eduard Matito Grass
Development of improved exchange-correlation functional.

Dr. David Casanova
Development, implementation and application of electronic structure methods for the study of electronic excited states and photophysical processes in molecules, aggregates and complex systems.

Seminars

09/01/2015
Water and water/metal interfaces from first principles.
Prof. Marivi Fernandez-Serra
Stony Brook University, New York, USA

13/01/2015
Detection of multipartite entanglement close to symmetric Dicke states.
Prof. Geza Giedke
Max-Planck-Institut für Quantenoptik, Garching, Germany

13/01/2015
Magnetic response of functionalized lipid bilayers.
Dr. Joachim Kohlbrecher
Paul Scherrer Institut, Villigen, Switzerland

14/01/2015
Hamiltonian adaptive QM/MM: multi-scale modeling of chemical reactions in solution.
Prof. Rosa Bulo
University of Utrecht, The Netherlands

15/01/2015
Direct growth of 2D materials on practical substrates: from surface chemistry to new physics and devices.
Prof. Jeffry A. Kelber
University of North Texas, Denton, USA

29/01/2015
Iatrochemistry, cannabis and drug design.
Prof. Pilar Goya Laza
Instituto de Química Médica (CSIC), Madrid, Spain

30/01/2015
Landscape without neutrinos.
Prof. Juan José Gómez-Cadenas
Instituto de Fisica Corpuscular CSIC-UV, Valencia, Spain

06/02/2015
Interactions between layers in ferroelectric superlattices.
Prof. Matthew Dawber
Stony Brook University, New York, USA

10/02/2015
Detecting quantum entanglement in multiparticle systems.
Dr. Geza Toth
Ikerbasque, Department of Theoretical Physics, UPV/EHU, Leioa, Spain

12/02/2015
Hunting for helical boundary states and Majoranas in superconductor-topological insulator-superconductor hybrid junctions.
Prof. Arturo Tagliacozzo
Università di Napoli Federico II, Napoli, Italy

13/02/2015
Quantum optics without photons from basic effects to new quantum information architectures.
Martin Schütz (PhD student)
MPQ Garching, Germany

16/02/2015
Contributions of Physics to Ethics: Nuclear Weapons, Free Will, and the Good Life.
Prof. Carl Mitcham
Colorado School of Mines, USA

16/02/2015
Electrical and thermal control of magnetic exchange interactions.
Prof. Jonas Fransson
Uppsala University, Sweden

18/02/2015
Chemical bonding in the light of an energy decomposition analysis.
Prof. Gernot Frenking
Fachbereich Chemie, Philipps Universität Marburg, Marburg, Germany

24/02/2015
Attosecond time-resolved photoemission experiments in cross comparison to spin resolved photoemission spectroscopy.
Prof. Ulrich Heinzmann
University of Bielefeld, Molecular & Surface Physics Bielefeld Institute for BioPhysics & NanoScience (BINAS) Bielefeld, Germany

25/02/2015
Attosecond electron dynamics in complex molecular systems.
Dr. Andrea Trabattoni
Politecnico di Milano, Milano, Italy

26/02/2015
Development of the PETAL laser facility and its applications in physics.
Prof. Dimitri Batani
Universitè de Bordeaux, Talence, France

27/02/2015
Rare earth doped fluoride materials for optics and photonics.
Prof. Michel Mortier
ParisTech, Ecole Nationale Superieure de Chimie de Paris, France

06/03/2015
Scanning tunneling spectroscopy of the superconducting vortex lattice.
Dr. Isabel Guillamon Gomez
Instituto de Ciencia de Materiales Nicolás Cabrera, Condensed Matter Physics Center, Universidad Autónoma de Madrid, Spain

09/03/2015
Nanostructured graphene: challenges in fabrication and modeling.
Prof. Antti-Pekka Jauho
Center for Nanostructured Graphene (CNG), DTU Nanotech,
Technical University of Denmark, Lyngby, Denmark

10/03/2015
Towards a chemically accurate description of reactive molecule-surface scattering.
Prof. Geert-Jan Kroes
Leiden Institute of Chemistry, Gorlaeus Laboratory, Leiden, The Netherlands

16/03/2015
Graphene-metal interaction revealed by scanning tunneling microscopy.
Dr. Hyowon Kim
Samsung Advanced Institute of Technology (SAIT) Yeoungtong-gu, Suwon-si, Korea

18/03/2015
La divulgación científica. Un cuento inexacto.
Dr. Ana Montserrat Rosell
TVE programa Tres14, Madrid, Spain

20/03/2015
Density functional theory based strategies for patterning and etching of semiconductor surfaces.
Dr. Sananda Biswas
International Centre for Theoretical Physica (ICTP), Trieste, Italy

25/03/2015
Step polymerization in various solvent conditions.
A computer simulation approach using “Patchy Brownian Cluster Dynamics”.
Dr. Jean-Christophe Gimel
Micro and Nano-medicine Laboratory, University Hospital in Angers, France

26/03/2015
Linear and nonlinear surface polaritons in graphene-based structures.
Prof. Yuliy Bludov
Center for Physics, University of Minho, Braga, Portugal

15/04/2015
Plasmons in nanographene and other atomic scale systems
Prof. Javier García de Abajo
ICFO-The Institute of Photonic Sciences, Castelldefels, Barcelona, Spain

24/04/2015
Strong field atomic ionization with linear and circular polarized light:
Spectra, cusps and time delay.
Prof. Anatoli Kheifets
Australian National University, Canberra, Australia

28/04/2015
ARPES insight into the dual nature of f- electrons in rare-earth intermetallics.
Prof. Denis Vyalikh
Dresden University of Technology, Dresden, Germany

29/04/2015
Exploring matter under extremes conditions at the linac coherent light source.
Eduardo Granados
SLAC Natioonal Accelerator Laboratory, Stanford University, California, USA

04/05/2015
Electronic and vibrational properties of $TiSe_2$ in the charge-density wave phase from first principles.
Dr. Raffaello Bianco
Paris VI (UPMC), France

08/05/2015
Beyond the Born-Oppenheimer approximation in matter under extreme conditions.
Prof. J. Alfredo Caro
Los Alamos National Laboratory, New Mexico, USA

19/05/2015
Basics and applications of nonlinear dielectric techniques.
Prof. Ranko Richert
Arizona State University, Tempe, USA

21/05/2015
Bound states in the continuum in graphene based nanostructure.
Prof. Luis Rosales Ahumada
Universidad Técnica Federico Santa María, Chile

22/05/2015
Outlook in neutrino physics.
Prof. Pilar Hernández Gamazo
Instituto de Física Corpuscular CSIC-UV, Valencia, Spain

29/05/2015
Quantum Engineering with ultracold matter.
Dr. Omjyoti Dutta
Jagiellonian University, Krakow, Poland

02/06/2015
Engineering of the electronic and opto-electronic properties of carbon nanotubes
via artificially induced defects and electrostatic doping.
Dr. Gilles Buchs
Swiss Center for Electronics and Microtechnology, CSEM, Switzerland

03/06/2015
Currrent topics in attosecond photoemission spectroscopy on metal surfaces and interfaces.
Dr. Martin Schäffer
Technische Universität München (TUM), Germany

05/06/2015
Charge transfer between donor-acceptor molecular networks on metal surfaces.
Dr. Jonathan Rodriguez Fernandez
IMDEA, Madrid, Spain

18/06/2015
Chemical Structures and mechanical properties of molecules studied by high-resolution foce microscopy.
Dr. Shigeki Kawai
University of Basel Switzerland PRESTO and Japan Science and Technology Agency, Kawaguchi, Japan

24/06/2015
Dopants acting as trap for electrons: Spin relaxation and decoherence.
Prof. María Chamarro Calvo
Pierre and Marie Curie University, Institut des NanoSciences de Paris, France

24/06/2015
Modelling colloidal semiconductor nanocrystals: towards realistic sizes.
Dr. Ivan Infante
Vrije Universiteit Amsterdam, The Netherlands

26/06/2015
k-resolved electronic structure by soft-X-ray ARPES:
From 3D systems to buried interfaces and impurities.
Dr. Vladimir N. Strokov
Swiss Light Source and Paul Scherrer Institute, Villigen-PSI, Switzerland

26/06/2015
Vibronic structure methods: from small molecules to systems with hundreds of atoms.
Prof. Robert Berger
Philipps-Universität Marburg, Germany

02/07/2015
Robust electron pairing in the integer quantum hall effect regime.
Prof. Moty Heiblum
Weizmann Institute of Science, Rehovot, Israel

06/07/2015
Simple design of topological state.
Dr. Xiao Hu
International Center for Materials Nanoarchitectonics (WPI-MANA)
National Institute for Materials Science (NIMS)
Tsukuba, Japan

21/07/2015
Quantum Optics in waveguides.
Prof. Luis Martín Moreno
Instituto de Ciencia de Materiales de Aragón, (ICMA), Zaragoza, Spain

22/07/2015
One electron reduced density matrix of strong correlation harmonium atom.
Dr. Jerzy Cioslowski
University of Szczecin, Poland

24/07/2015
Electrical contacts to two-dimensional materials: when less is more.
Dr. Xavier Cartoixà Soler
Universidad Autónoma de Barcelona, Spain

30/07/2015
STM-based spectroscopies of single-molecule and single-atom contacts.
Richard Berndt
Institute of Experimental and Applied Physics, University of Kiel, Germany

04/08/2015
Manipulation of the induced pair potential in topological insulator-superconductor hybrid junctions.
Dr. Pablo Burset Atienza
University of Würzburg, Germany

07/08/2015
Mesoscopic and nonequilibrium superconductivity in nanohybrids.
Prof. Teunis Klapwijk
Delft University of Technology, The Netherlands

11/09/2015
Many-body interaction induced exotic phenomena at surface: molecular Kondo effect and inelastic process in laser-photoemission.
Prof. Emi Minamitani
Graduate School of Engineering
The University of Tokyo, Bunkyo-ku, Tokyo, Japan

18/09/2015
Novel 2D electron gases at the surface of transition-metal oxides.
Prof. Andres Felipe Santander Syro
CSNSM, Université Paris-Sud, France

22/09/2015
CO_2 capture in aqueous solutions: insights from ab initio simulations.
Prof. Wanda Andreoni
Ecole Polytechnique Federale de Lausanne, EPFL Institute of Theoretical Physics, Lausanne, Switzerland

30/09/2015
Understanding the stiffness of Macromolecules: From single chains to semi flexible polymer brushes.
Prof. Kurt Binder
Johannes Gutenberg University, Mainz, Germany

06/10/2015
La labor de la Fundación Española para la Ciencia y la Tecnología: participación social en la ciencia.
Prof. José Ignacio Fernandez Vera
FECYT, Madrid, Spain

09/10/2015
Atomic clocks and other marvels of absolute frequency measurements.
Prof. Amand Lucas
University of Namur, Belgium

21/10/2015
The role of short-range order and hyperuniformity in the formation of band gaps in 2D disordered photonic materials.
Dr. Luis Froufe Perez
University of Fribourg, Switzerland

22/10/2015
Single-atom optical clocks.
Prof. David Jeffery Wineland
NIST, Boulder, Colorado, USA

29/10/2015
Image processing tools for the study of brain connections.
Dr. Ignacio Arganda Carreras (Ikerbasque Fellow)
University of the Basque Country, UPV/EHU, Spain

06/11/2015
Hybrid upconversion nanomaterials for photochemotherapy.
Luca Salassa
CIC BiomaGUNE, Donostia/San Sebastián, Spain

11/11/2015
Stellar occultations: Chariklo and its ring system.
Rodrigo Leiva
Instituto de Astrofísica, Facultad de Física, Pontificia Universidad Católica de Chile.
Observatoire de Paris, LESIA, France

19/11/2015
Topologically confined states at corrugations of gated bilayer graphene.
Dr. Marta Pelc
CFM, Centro de Física de Materiales, Donostia/San Sebastián, Spain

15/12/2015
100 años de Relatividad General.
Prof. Alberto Galindo Teixaire
Ex-Presidente de la Real Academia de Ciencias Exactas, Físicas y Naturales

Workshops

Theory for Planar Molecular and Atomic Scale Devices

January 26-28, 2015
Donostia International Physics Center, Donostia/San Sebastián
http://dipc.ehu.es/ws_presentacion.php?id=116

Organizing Committee
Daniel Sánchez-Portal (CFM CSIC-UPV/EHU, DIPC)
Mads Engelund (CSIC, Madrid)
Thomas Frederiksen (DIPC, Ikerbasque)
Aran García-Lekue (DIPC, Ikerbasque)

The aim of the workshop was to bring together some of the groups working actively on the field (singularly those involved in the European Integrated Fp7 FET project PAMS, contract number 610446). The explored atomic and molecular devices included dangling bond circuitries, functionalized by coupling with organic molecules, and controlled by remote alteration of molecular states by local band bending. Multibranch polyaromatic logical gates addressed by nanowires were also explored.
The development of new methodological tools, allowing for a multiscale description (using from first-principles to empirical force-fields) of the structural, electronic and transport properties of such atomic and molecular devices was also discussed. The ultimate aim was to optimize the design and synthesis of atomic and molecular gates by developing these new theoretical tools.

Invited Speakers

Ville Loukonen, Hugo Pinto, Juha Ritala, John Tracey and Adam Foster (Aalto University)

Mads Engelund from (CSIC)

Thomas Frederiksen (Ikerbasque, DIPC)

Benoit Eydoux, Ghassen Dridi, Omid Faizy (CEMES-CNRS, Toulouse)

Andrii Kleshchonok, Thomas Lehmann (Dresden University of Technology)

Daniel Sánchez-Portal (CFM CSIC-UPV/EHU, DIPC)

Imaginenano 2015

March 10-13, 2015
Bilbao Exhibition Center - BEC
www.imaginenano.com

Organizers
Phantoms Foundation, CIC nanoGUNE, DIPC, CFM, UPV/EHU and BEC

The 3rd edition of the largest European Event in Nanoscience & Nanotechnology, ImagineNano, gathered the global nanotechnology community, including researchers, industry policymakers and investors. Following the overwhelming success of ImagineNano 2013, several conferences were held in parallel in a new infrastructure, as well as a vast exhibition, one-to-one meetings and an industrial forum where everyone could meet and greet Nanotechnology side by side.

Five different conferences on Nanoscience & Nanotechnology were organized covering hot topics in the fields of Graphene, Bio/Medicine, Optics, Photonics, Chemistry, and Toxicology.

Key Lectures

Ignacio Cirac (Max Planck Institute of Quantum Optics, Germany)

Jean Marie Lehn (University of Strasbourg, France)

Discussions on Nano and Mesoscopic Optics (DINAMO) 2015

April 8-12, 2015
El Chalten (Santa Cruz, Argentina)
http://dinamo2015.df.uba.ar/

Organizing Committee
Andrea Bragas (CONICET, UBA, Argentina)
Marcelo Lester (UNICEN, Tandil, Argentina)
Stefan A. Maier (Imperial College London, UK)
Juan José Sáenz (UAM, Madrid and DIPC, San Sebastián, Spain)
Fernando Stefani (CONICET, UBA, Argentina)

Scientific Committee
Javier Aizpurua (CFM CSIC-UPV/EHU, DIPC, San Sebastián, Spain)
Aristide Dogariu (CREOL, Florida, USA)
Lukas Novotny (ETH-Zürich, Switzerland)
Gabriel Cwilich (Yeshiva University, NY, USA)
Markus Schmidt (Friedrich Schiller University Jena, Germany)

The subjects covered by DINAMO embraced practically all branches of nano- and mesoscopic optics, including plasmonics, optical manipulation, cavity optics, optical fields in random media, single molecule spectroscopy, non-linear nano-optics, nano-holography, optical nano-antennas, opto-mechanics and bio-photonics, both from experimental and theoretical viewpoints.

DINAMO was conceived to provide an interdisciplinary forum where leading investigators from around the world could present and discuss their latest work and future challenges in an informal and interactive format.

Invited Speakers

Guillermo Acuña (Technische Universität Braunschweig, Germany)

Jeremy Baumberg (Cambridge University, UK)

Remi Carminati (Institut Langevin, ESPCI, France)

Scott Carney (University of Illinois at Urbana-Champaign, USA)

Eduardo Coronado (University of Córdoba, Argentina)

Alejandro Fainstein (Instituto Balseiro, Argentina)

Jochen Feldman (LMU Munich, Germany)

Mathias Fink (Institut Langevin, France)

Monika Fleischer (Universität Tübingen, Germany)

Ernst-Ludwig Florin (University of Texas at Austin, USA)

P. David Garcia (University of Copenhagen, Denmark)

Francisco J. Garcia Vidal (IFIMAC, Universidad Autónoma de Madrid, Spain)

Rainer Hillenbrand (Nanogune, Spain)

Ulrich Hohenester (University of Graz, Austria)
Christiane Höppener (University of Münster, Germany)
Peter Johansson (Chalmers, Sweden)
Mikael Käll (Chalmers, Sweden)
Stephane Kena-Cohen (Imperial College/Polytechnique Montreal, Canada)
Pieter Kik, CREOL (University Central Florida, USA)
Daniel Lanzillotti Kimura (Laboratoire de Photonique et de Nanostructures, France)
Cefe López (ICMM-CSIC, Spain)
John Lupton (Universität Regensburg, Germany)
Onofrio M. Marago, (CNR-IPCF, Italy)
Georg Maret (Konstatz University, Germany)
Oscar Martínez (Universidad de Buenos Aires, Argentina)
Gabriel Molina-Terriza (Macquarie University, Australia)
Otto Muskens (University of Southampton, UK)
Manuel Nieto-Vesperinas (ICMM-CSIC, Spain)
Jose Ignacio Pascual (CIC nanoGUNE, Spain)
Francesco Pedaci (Centre de Biochimie Structurale, Montpellier, France)
Helmut Ritsch (University of Innsbruck, Austria)
Monika Ritsch-Marte (Innsbruck Medical Univ., Austria)
Halina Rubinsztein (University of Queensland, Australia)
Frank Scheffold (University of Fribourg, Switzerland)
Norbert F. Scherer (University of Chicago, USA)
Sergey Skipetrov (CNRS, Grenoble, France)
Galo Soler-Illia (University of Buenos Aires, Argentina)
Philip Tinnefeld (Technische Universität Braunschweig, Germany)
Niek van Hulst (ICFO, Barcelona, Spain)
Silvia Vignolini (University of Cambridge, UK)
Alex Weber-Bargioni (Material Science Devision LBNL, Berkeley, USA)
Ulrike Woggon (TUB Berlin, Germany)
Pavel Zemanek (Institute of Scientific Instruments, Academy of Sciences, Czech Republic)

11th Capri Spring School on Transport in Nanostructures 2015

April 12-19, 2015
Villa Orlandi, Isola di Capri, Italy
www.capri-school.eu

Organizing Committee
Dario Bercioux (Ikerbasque, DIPC)
Alessandro De Martino (City University London)
Reinhold Egger (Heinrich-Heine-Universität - Düsseldorf)
Hermann Grabert (Albert-Ludwig-Universität - Freiburg)
Christian Schönenberger (Universität Basel)
Arturo Tagliacozzo (Università "Federico II" Napoli)

This one week spring school on topological superconductivity provided several three to four hour lectures by leading experts supplemented by a few shorter seminars. The speakers gave graduate level presentations introducing state-of-the-art methods and techniques featuring the key issues of the field of topological superconductivity. While the school was primarily aimed at instructing PhD students and young postdoctoral researchers, more senior scientists who wanted to acquaint themselves with the subject of the school were also welcome.

Keynote Speakers
Yoichi Ando (Osaka)
Liang Fu (MIT)
Moty Heiblum (Weizmann)
Tony Leggett (Urbana)
Andreas Schnyder (MPI Stuttgart)
Björn Trauzettel (Würzburg)

The 15th International Conference on Vibrations at Surfaces (VAS15)

June 22-26, 2015
Miramar Palace, Donostia/San Sebastián
http://vas15.dipc.org/

Organizing Committee
Andres Arnau (CFM CSIC-UPV/EHU, DIPC)
Giorgio Benedek (Università degli Studi di Milano)
Eugene Chulkov (UPV/EHU, DIPC)
Asier Eiguren (UPV/EHU)
Aran Garcia Lekue (DIPC, Ikerbasque)
Aitor Mugarza (ICN2)
Jose Ignacio Pascual (CIC nanoGUNE, Ikerbasque)
Thomas Frederiksen (DIPC, Ikerbasque) (Chair)

International Advisory Committee
Philip B. Allen, Stony Brook (USA)
Heriberto Fabio Busnengo, CONICET Rosario (Argentina)
Renée D. Diehl, Penn State (USA)
Ricardo Diez Muiño, CFM –CSIC-UPV/EHU– and DIPC (Spain)
Claudia Draxl, Humboldt University Berlin (Germany)
Karl-Heinz Ernst, EMPA (Switzerland)
Wolfgang Ernst, TU Graz (Austria)
Daniel Farías, Universidad Autónoma de Madrid (Spain)
Hans-Joachim Freund, Fritz-Haber-Institut der MPG, Berlin (Germany)
Wilson Ho, University of California-Irvine (USA)
Chakram S. Jayanthi, University of Louisville (USA)
Maki Kawai, University of Tokyo (Japan)
Zhiyuan Li, Chinese Academy of Sciences, Beijing (China)
Nicolas Lorente, CIN2 Barcelona (Spain)
Joseph R. Manson, Clemson University (USA)
Richard E. Palmer, University of Birmingham (UK)
Talat S. Rahman, University of Central Florida (USA)
Mario Rocca, Universitá Genova (Italy)
Erio Tosatti, SISSA Trieste (Italy)
Hiromu Ueba, University of Toyama (Japan)

Vibrations at Surfaces (VAS) was an international conference and main venue for scientific exchange in the field of surface vibrational spectroscopy and surface dynamics. VAS15 covered topics such as:

Dynamics at surfaces
Electron and thermal transport
Nanotribology and friction
STM-IETS
Surface chemistry and catalysis
Surface scattering
Time-resolved vibrational spectroscopy
Tip-enhanced Raman spectroscopy
Topological insulators and superconductors
Vibrations of 2D structures and layered materials

Invited Speakers
Ellen Backus (MPI Mainz, Germany)
Rainer Beck (EPFL, Switzerland)
Marie-Laure Bocquet (ENS Montrouge, France)
Matteo Calandra (Université Pierre et Marie Curie, Paris, France)
Kramer Campen (FHI Berlin, Germany)
Davide Donadio (DIPC, Spain)
Zhenchao Dong (USTC Hefei, China)
Michael El-Batanouny (Boston University, USA)
John Ellis (University of Cambridge, United Kingdom)
M. Verónica Ganduglia-Pirovano (ICP CSIC, Madrid, Spain)
Karsten Hannewald, (Humboldt-University, Berlin, Germany)
Holly Hedgeland (UCL, United Kingdom)
Peter Jakob (Marburg University, Germany)
Ying Jiang (Peking University, China)
Yousoo Kim (RIKEN Tokyo, Japan)
Nicolas Lorente (CFM-CSIC, DIPC, Spain)
John Polanyi (University of Toronto, Canada)
Mark A. Reed (Yale University, USA)
Jascha Repp (Regensburg University, Germany)
Irina Y. Sklyadneva, (DIPC and Tomsk State University)
Sergio O. Valenzuela (Institut Catala de Nanociencia i Nanotecnologia, Spain)
Richard P. Van Duyne (Northwestern University, USA)
Justin Wells (NTNU, Norway)
Alec M. Wodtke (MPI Göttingen, Germany)

New Trends in Topological Insulators 2015 (NTTI2015)

July 6-10, 2015
Miramar Palace, Donostia/San Sebastian
http://dipc.ehu.es/ws_presentacion.php?id=110

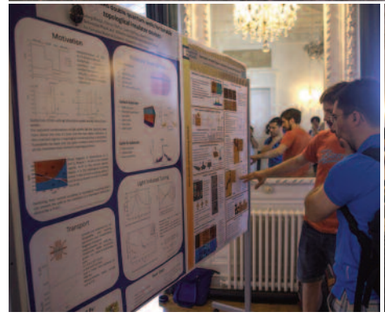
Scientific Committee
Evgueni V. Chulkov (UPV/EHU, DIPC)
M. Zahid Hasan (Princeton University, USA)
Laurens Molenkamp (University of Würzburg, Germany)
Sergey Frolov (University of Pittsburg)

Organizing Committee
Evgueni V. Chulkov (UPV/EHU, DIPC)
Maia G. Vergniory (DIPC)
Mikhail M. Otrokov (DIPC)

New Trends in Topological Insulators (NNTI) is an international conference and main venue for scientific exchange in the field of Topological Insulators in Europe. NTTI2015 is the third edition of a series of meetings that started a few years ago in Saint Feliu de Guixols (2013) and Berlin (2014).

As in the previous meetings the goal of NTTI2015 was to bring together experienced and young researchers as well as students working in topological insulators from different aspects, such as magnetic interaction, collective excitations, superconductivity, quantum anomalous hall effect and electron and spin structure.

Invited speakers
B. Andrei Bernevig (Princeton University, USA)
Gustav Bihlmayer (Forschungszentrum Jülich, Germany)
Sergey Eremeev (Russian Academy of Sciences, Moscow, Russia)
Arthur Ernst (Max Planck Institute of Microstructure Physics, Germany)
Motohiko Ezawa (University of Tokyo, Japan)
Sergey Frolov (University of Pittsburgh, USA)
Zahid Hasan (Princeton University, USA)
Rolph Heid (Karlsruher Institut für Technologie, Germany)
Akio Kimura (Hiroshima University, Japan)
Holger Meyerheim (Max Planck Institute of Microstructure Physics, Germany)
Laurens Molenkamp (University of Würzburg, Germany)
Jagadeesh Moodera (MIT, USA)
Herbert Pfnur (Leibniz Universität Hannover, Germany)
Antonio Politano (Università degli Studi della Calabria, Italy)
Oliver Rader (Helmholtz Zentrum, Berlin, Germany)
Andreas Schnyder (Max-Planck-Institut für Festkörperforschung, Germany)
Jonathan Sobota (Stanford University, USA)
Ilya Sochnikov (Stanford University, USA)
Marin Soljacic (MIT, USA)
Yukio Tanaka (Nagoya University, Japan)
Alexey Taskin (Nagoya University, Japan)
Christoph Tegenkamp (Leibniz Universität Hannover, Germany)
Atsushi Tsukazaki (Tohoku University, Japan)
Tonica Valla (Brookhaven National Laboratory, USA)
Bohm-Jung Yang (RIKEN Center for Emergent Matter Science, Japan)
Ali Yazdani (Princeton University, USA)
Oleg Yazyev (EPFL, Switzerland)



Interaction effects in graphene and related materials

July 13-17, 2015
Miramar Palace, Donostia/San Sebastian
http://dipc.ehu.es/iegr/

Organizing Committee
Andres Arnau (CFM CSIC-UPV/EHU, Donostia/San Sebastian, Spain)
Paco Guinea (University of Manchester, UK, and Imdea Nanoscience, Madrid, Spain)
Rainer Hillenbrand (CIC nanoGUNE, Ikerbasque, San Sebastian, Spain)
Rodolfo Miranda (Imdea Nanoscience, Madrid, Spain)
Vittorio Pellegrini (IIT, Genoa, Italy)
Marco Polini (Scuola Normale Superiore, Pisa, Italy)

The workshop focused on "interaction effects" in graphene and related materials including hexagonal boron nitride, transition metal dichalcogenides, and few-layer black phosphorus. This workshop covered recent advances in our understanding of fundamental interactions in 2D materials and their van der Waals stacks, with top-notch speakers spanning a wide variety of cryogenic and non-cryogenic phenomena that emerge in magneto-transport, linear and non-linear optics, plasmonics, and spintronics spectroscopies.

Invited Speakers
E. Andrei (New Jersey, USA)
R. Asgari (Tehran, Iran)
R. Ashoori (Massachussetts, USA)
D. Basov (California, USA)
G. Bilhmayer (Jülich, Germany)
M. Bockrath (California, USA)
K. Bolotin (Tennessee, USA)
I. Brihuega (Madrid, Spain)
A. Castellanos (Madrid, Spain)
A.H. Castro Neto (Singapore)
M.A. Cazalilla (Taiwan)
S. Das Sarma (Maryland, USA)
K. Ensslin (Zurich, Switzerland)
V.I. Fal'ko (Lancaster, UK)
J. Fernandez-Rossier (Braga, Portugal)
A.C. Ferrari (Cambridge, UK)
A. Fert (Saclay, France)
M. Fogler (California, USA)
A. Geim (Manchester, UK)
J. Gomez (Madrid, Spain)
Chema Gómez (Madrid, Spain)
C. Gomez-Navarro (Madrid, Spain)
J. Gonzalez (Madrid, Spain)
I. Grigorieva (Manchester, UK)
I. Herbut (Columbia, Canada)
P. Jarillo-Herrero (Massachussetts, USA)
M.I. Katsnelson (Neijmegen, The Netherlands)
F.H.L. Koppens (Barcelona, Spain)
A. Lanzara (California, USA)
J. Lau (California, USA)
L. Levitov (Massachussetts, USA)
S.G. Louie (California, USA)
T. Low (Minnesota, USA)
A.H. MacDonald (Texas, USA)
H. Manoharan (California, USA)
L. Martin-Moreno (Zaragoza, Spain)
N. Marzari (Lausanne, Switzerland)
F. Mauri (Paris, France)
Ygal Meir (Negev, Israel)
E. Mele (Pennsylvania, USA)
G. Montanbaux (Paris, France)
A. Morpurgo (Geneve, Switzerland)
B. Narozhny (Karlsruhe, Germany)
H. Ochoa (California, USA)
B. Özyilmaz (Singapore)
Nuno Peres (Braga, Portugal)
L. Ponomarenko (Lancaster, UK)
M. Potemski (Grenoble, France)
S. Roche (Barcelona, Spain)
E. Rossi (Virginia, USA)
E. Rotenberg (California, USA)
P. San Jose (Madrid, Spain)
C. Stampfer (Aachen, Germany)
Efrat Shimsoni (Tel Aviv, Israel)
Bart van Wees (Groningen, The Netherlands)
A. Vazquez de Parga (Madrid, Spain)
G. Vignale (Missouri, USA)
M. Vozmediano (Madrid, Spain)
A. Yacoby (Massachussetts, USA)

HQ-4. Fourth Conference on the History of Quantum Physics

July 15-18, 2015
Miramar Palace, Donostia/San Sebastian
www.ehu.eus/en/web/hq-4/home

Organizing/Scientific Committee
Alexander Blum (Max Planck Institute for the History of Science)
Christian Joas (Ludwig Maximilian Universität, München)
Christoph Lehner (Max Planck Institute for the History of Science)
Jaume Navarro (University of the Basque Country and Ikerbasque)
Jurgen Renn (Max Planck Institute for the History of Science)
Iñaki San Pedro (University of the Basque Country)

The last decade saw a surge in new scholarship on the history of quantum physics, built upon new sources, interpretations, and historiographical approaches. Three successful meetings in Berlin (2007), Utrecht (2008) and Berlin (2010) triggered a momentum of innovative projects and novel publications on the topic, which this conference followed and expanded upon. The Donostia International Physics Center (DIPC) and the Max Planck Institute for the History of Science (MPIWG) jointly organized the fourth edition of this series of conferences in Donostia/San Sebastian.

The meeting gathered scholars working on the history of quantum physics broadly understood from as many points of view as possible: from the conceptual to the sociological, from the institutional to the philosophical, from the academic to the popular.

Invited Speakers
Clayton A. Gearhart (St. John's University)
Blai Pié i Valls & Enric Pérez Canals (U. Barcelona)
Martha Cecilia Bustamante (U. Paris Diderot)
Arne Schirrmacher (Humboldt Universität)
Giora Hon (U Haifa)
Anthony Duncan & Michel Janssen (U Minnesota)
Martin Jähnert (MPIWG)
Christoph Lehner, Alex Blum, Martin Jähnert & Jurgen Renn (MPIWG)
Gonzalo Gimeno (U Autònoma Barcelona)
Nicolás Gaudenzi (UNAM)
Guido Bacciagaluppi & Elise (Crull & Owen Maroney)
Alexei Kojevnikov (UBC)
Alex Blum (MPIWG)
Aaron Sidney Wright (Harvard University)
Dennis Dieks (U Utrecht)
Arianna Borrelli (TU)
Alessio Rocci (U. of Padova)
María C. Boscá (U. of Granada)
Jean-Philippe Martinez (U. Paris Diderot)
Christian Joas (LMU)
Andrew Zangwill (Georgia Institute of Technology)
Kenji Ito (The Graduate University for Advanced Studies (Sokendai))
Asim Gangopadhyaya & Aleksandr Goltsiker. (U. of Loyola)
Roberto Lalli (MPIWG)
Shaul Katzir (U. of Tel Aviv)
Daniela Monaldi (York University)
An Rettig (U. of Regensburg)
Virgile Besson (U. Claude Bernard Lyon 1)
Thiago Hartz (Niels Bohr Archive)
Olival Freire Jr (Universidade Federal da Bahia)

International Symposia on (e,2e), Double Photo-ionization and Related Topics & Polarization and Correlation in Electronic and Atomic Collisions

July 30 - August 1, 2015
Miramar Palace, Donostia/San Sebastián
http://e2epol.dipc.org/

Chairmen
Ricardo Díez Muiño (DIPC, CFM CSIC-UPV/EHU)
Nikolay M. Kabachnik (Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University)

The *International Symposium on (e,2e), Double Photo-ionization and Related Topics* and the *18th International Symposium on Polarization and Correlation in Electronic and Atomic Collisions* were organized in San Sebastian as official satellite meetings of *ICPEAC 2015*. The merging of the two symposia into a single scientific event provided the opportunity to attend high-level specialized talks covering a broad range of hot topics in atomic and molecular physics. Among others, the following problems were discussed:

• Many-body interactions and electron-electron correlation effects in single and multiple ionization processes.
• Alignment and polarization effects in excitation and charge transfer processes.

International Scientific Committee
Ugo Ancarani (Université de Lorraine, Metz, France)
Lorenzo Avaldi (CNR-IMIP, Rome, Italy)
Klaus Bartschat (Drake University, Des Moines IA, USA)
Jamal Berakdar (Martin-Luther-Universität Halle-Wittenberg, Germany)
Nora Berrah (University of Connecticut, Storrs CT, USA)
Igor Bray (Curtin University, Perth, Australia)
Michael Brunger (Flinders University, Adelaide, Australia)
Xiangjun Chen (University of Science and Technology, Hefei, Anhui, China)
James Colgan (Los Alamos National Laboratory, Los Alamos NM, USA)
Alexander Dorn (Max-Planck-Institut für Kernphysik, Heidelberg, Germany)
Reinhard Dörner (Goethe-Universität, Frankfurt am Main, Germany)
Danielle Dowek (Université Paris Sud, Orsay, France)
Omar Ariel Fojón (Instituto de Física Rosario, Argentina)
Timothy Gay (University of Nebraska – Lincoln NE, USA)
Alexei N. Grum-Grzhimailo (Lomonosov Moscow State University, Moscow, Russia)
Nikolay Kabachnik (Lomonosov Moscow State University, Moscow, Russia)
Anatoli Kheifets (Australian National University, Canberra, Australia)
Murtadha Khakoo (California State University, Fullerton CA, USA)
George King (University of Manchester, UK)
Tom Kirchner (York University, Toronto, Canada)
Noriyuki Kouchi (Tokyo Institute of Technology, Tokyo, Japan)
Don H. Madison (Missouri S&T, Rolla MO, USA)
Fernando Martín (Universidad Autónoma de Madrid, Spain)
Michael Meyer (European XFEL, Hamburg, Germany)
Andrew Murray (University of Manchester, UK)
Roberto Rivarola (Instituto de Física Rosario, Argentina)
Michael Schulz (Missouri S&T, Rolla MO, USA)
Rajesh Srivastava (Indian Institute Of Technology Roorkee, Uttarakhand, India)
Al Stauffer (York University, Toronto, Canada)
Emma Sokell (University College Dublin, Ireland)
Masahiko Takahashi (Tohoku University, Sendai, Miyagi, Japan)
Kiyoshi Ueda (Tohoku University, Sendai, Miyagi, Japan)
Joachim Ulrich (Max-Planck-Institut für Kernphysik, Heidelberg, Germany)
Jim Williams (University of Western Australia, Perth, Australia)
Akira Yagishita (Photon Factory, Tsukuba, Japan)

Local Organizing Committee
Maite Alducin Ochoa (Centro de Física de Materiales CSIC-UPV/EHU & DIPC, Donostia/San Sebastián)
María Blanco-Rey (Departamento de Física de Materiales UPV/EHU & DIPC, Donostia/San Sebastián)
Iñaki Juaristi Oliden (Centro de Física de Materiales CSIC-UPV/EHU & DIPC, Donostia/San Sebastián)
Mohammed Ahmed Nosir (Centro de Física de Materiales CSIC-UPV/EHU, Donostia/San Sebastián)

Plenary Lecturers
Lorenz Cederbaum (University of Heidelberg, Germany)
Anatoli Kheifets (Australian National University, Canberra, Australia)
Giovanni Stefani (Università di Roma Tre, Rome, Italy)

Invited Speakers
Ugo Ancarani (Université de Lorraine, Metz, France)
Lorenzo Avaldi (CNR - Istituto di Struttura della Materia, Roma, Italy)
Klaus Bartschat (Drake University, Des Moines IA, USA)
Xiangjun Chen (University of Science and Technology, Hefei, Anhui, China)
James Colgan (Los Alamos National Laboratory, Los Alamos NM, USA)
Alexander Dorn (MPI für Kernphysik, Heidelberg, Germany)
Li Fang (University of Texas, Austin, TX USA)
Andreas Fischer (MPI für Kernphysik, Heidelberg, Germany)
Daniel Fischer (MPI für Kernphysik, Heidelberg, Germany)
Omar Ariel Fojon (Instituto de Física de Rosario, Argentina)
John Furst (University of Newcastle, Ourimbah, Australia)
Renaud Guillemin (Université Pierre et Marie Curie, Paris, France)
Leigh Hargreaves (California State University, Fullerton CA, USA)
Andrey Kazansky (Donostia International Physics Center, Donostia/San Sebastián, Spain)

Allen Landers (Auburn University AL, USA)
Don H. Madison (Missouri S&T, Rolla MO, USA)
Nicholas Martin (University of Kentucky, Lexington KY, USA)
Tommaso Mazza (European XFEL, Hamburg, Germany)
Laurent Nahon (SOLEIL Synchrotron, Gif-sur-Yvette, France)
Kyo Nakajima (JASRI, Hyogo, Japan)
Christophe Nicolas (SOLEIL Synchrotron, Gif-sur-Yvette, France)
Alicia Palacios (Universidad Autónoma de Madrid, Spain)
Béla Paripás (University of Miskolc, Hungary)
Artem Rudenko (Kansas State University, Manhattan, KS, USA)
Kirsten Schnorr (MPI für Kernphysik, Heidelberg, Germany)
Michael Schulz (Missouri S&T, Rolla MO, USA)
Olga Smirnova (Max Born Institute, Berlin, Germany)
Emma Sokell (University College Dublin, Ireland)
Al Stauffer (York University, Toronto, Canada)
Andrey Surzhikov (Helmholtz-Institut Jena, Germany)
Kiyoshi Ueda (Tohoku University, Sendai, Miyagi, Japan)
Oleg Vasyutinskii (Ioffe Physical Technical Institute, St. Petersburg, Russia)
Masakazu Yamazaki (Tohoku University, Sendai, Miyagi, Japan)
Shaofeng Zhang (Institute of Modern Physics, Lanzhou, China)

Workshop MANA–DIPC
"Nanostructures and Complex Functional Materials"

August 27-28, 2015
Donostia International Physics Center, Donostia/San Sebastián
http://dipc.ehu.es/ws_presentacion.php?id=123

Chairmen
Yutaka Wakayama (MANA)
Enrique Ortega (UPV/EHU, CFM CSIC-UPV, DIPC)

Workshop organized within the framework of the collaboration agreement between DIPC and the International Center for Materials Nanoarchitectonics (MANA) in Japan.

PRESENTATION

Prof. Pedro M. Echenique (UPV/EHU, DIPC)
Prof. Masakazu Aono (MANA)

NANOPHOTONICS SESSION

Tadaaki Nagao - MANA
Plasmonic Nanoarchitectonics for Energy Conversion

Javier Aizpurua - CFM CSIC-UPV/EHU, DIPC
Quantum effects in the optical response of plasmonic nano-antennas

Rainer Hillenbrand - CIC nanoGUNE, Ikerbasque
Nanoimaging and manipulation of plasmons in graphene

Peter Koval - DIPC
Ab-initio spectroscopy of large quantum systems

Atsushi Kubo - MANA
Evolution of surface plasmon wave packets in femtosecond time-domain

Yury Rakovich - CFM CSIC-UPV/EHU, Ikerbasque
Enhancement effects in hybrid organic/inorganic nanosystems: from resonant energy transfer to strong coupling

Ruben Esteban - DIPC
Topological insulator systems and strong coupling in light-matter interactions

SURFACES AND INTERFACES

Nacho Pascual - CIC nanoGUNE, Ikerbasque
The temperature of a single-molecule junction

Yoichi Yamada - MANA
Molecular-Scale and Macroscopic Properties of Organic Films

Iñaki Juaristi - CFM CSIC-UPV/EHU
Gas-Surface Dynamics Simulations

Yutaka Wakayama - MANA
STM study on solid-state reactions in binary molecular assemblies

Remi Petuya - DIPC
Bipolar conductance switching of anthraditionphene molecules

Seunjun Oh - MANA
Characterization and engineering of hybrid polymer-oxide semiconductor heterointerface

Guillaume Vasseur - DIPC
Full one-dimensional band dispersion in polymeric nanowires

Daniel Sánchez-Portal - CFM CSIC-UPV/EHU, DIPC
Semiconductor Surfaces: modelling from first principles

Takahiro Nagata - MANA
Crystallographic polarity effect of oxide on π conjugated system

Duncan Mowbray - DIPC
GW and BSE at the Interface: H_2O, CH_3OH, and Catechol on TiO_2

Tomoko Shimizu - MANA
Imaging Three-dimensional Surface Objects with Submolecular Resolution by Atomic Force Microscopy

Emilio Artacho - CIC nanoGUNE, Ikerbasque
Theoretical approaches to electrons in oxide surfaces

Yoshiyuki Yamashita - MANA
Hard X-ray Photoelectron Spectroscopy for Characterization of Advanced Materials

Celia Rogero - CFM CSIC-UPV/EHU
On the interfacial properties of solar cells

TRANSPORT IN NANOSTRUCTURES SESSION

Masakuzu Aono - MANA
Observing the transport of electrons, polarons and ions at the nanometer scale

Thomas Frederiksen - DIPC, Ikerbasque
First-principles simulations of transport in nanoelectronics

Aran Garcia-Lekue - DIPC, Ikerbasque
Structural, electronic and transport properties of graphene nanostructures

Ion Errea - UPV/EHU, DIPC
Vibrational and superconducting properties of transition metal dichalcogenides from first-principles

Dario Bercioux - DIPC
Scattering Properties of Defected Carbon-Nanotubes

Miguel Cazalilla: National Tsing Hua University, DIPC
Spin Hall Effects in Graphene and Two-Dimensional Materials

Takashi Uchihashi - MANA
Surface Superconductors on Silicon: Atomic-Step Josephson Junctions and Molecular Hybrid Materials

Sebastian Bergeret - CFM CSIC-UPV/EHU, DIPC
Spin-dependent transport in superconducting hybrid structures

Misha Otrokov - DIPC
Magnetic interactions at Ferromagnets/Topological Insulators interfaces

Summer School "Frontiers of Condensed Matter 2015"

August 31–September 11, 2015
Les Houches (France)
http://dipc.ehu.es/ws_presentacion.php?id=119

Organizing Committee
S. Bergeret (CFM CSIC-UPV/EHU, DIPC)
F. Hekking (Université Joseph Fourier, Grenoble)
J. Meyer (Université Joseph Fourier, Grenoble)
J. van Ruitenbeek (Leiden University)

This doctoral training session was organized jointly by the Physics Graduate School of Grenoble, by the Casimir Research School of Delft – Leiden (Netherlands) and the Donostia International Physics Center (DIPC) of San Sebastian (Spain). It aimed at offering final year Master students and junior Ph.D-students (1st/2nd year) a high-level training programme in the general area of condensed matter physics.

The session intended for experimentalists and theoreticians consisted of a series of pedagogical lectures, complemented by more specialized research seminars on timely topics. During the session, there was plenty of time for informal discussions between participants and lecturers. A poster session was organized, including a short oral presentation at the beginning of the session enabling the participants to present their research interests to each other.

Lecturers & Topics
S. Bergeret (CFM CSIC-UPV/EHU, DIPC) Spin-dependent transport in hybrid systems
J. Meyer (Université de Grenoble Alpes) Topological phases
Yu. Nazarov (Delft University of Technology, Université de Grenoble) Quantum Transport
J. Pekola (Aalto University, Université de Grenoble) Quantum thermodynamics
F. Pistolesi (Université de Bordeaux) Nanomechanics
L. Fritz (Utrecht University) Strongly correlated systems

Seminar Speakers
D. Basko (Université de Grenoble)
C. Bäuerle (Université de Grenoble)
P. Brouwer (Freie Universität Berlin)
F. Giazotto (Scuola Normale Superiore di Pisa)
R. Hanson (Delft University)
F. Hekking (Université de Grenoble)
J. van Ruitenbeek (Leiden University)
V. Vitelli (Leiden University)

The Ψk 2015 Conference

September 6-10, 2015
Kursaal Congress Centre, Donostia/San Sebastian
http://nano-bio.ehu.es/psik2015/

Organizing Committee
Angel Rubio (UPV/EHU, Max Planck, DIPC)
Risto Nieminen (Aalto University School of Science)

The **Ψ**k 2015 Conference is the fifth in a series started in 1996 by the European electronic structure community. Every five years, this conference brings together the global community that is active in the science of electronic structure and properties of condensed matter. The conference is organized and supported by the Psi-k Network, and its programme covers both the fundamental and theoretical aspects of electronic structure calculations, computational methods and tools, in addition to applications to fundamental scientific and industrial and societal challenges. The application areas of electronic property calculations ranged from condensed matter and materials physics to nanoscience, chemistry, geophysics and biology, the design and discovery of novel materials, their properties, and their performance in devices (that is, to harvest, store, and convert energy) and to engineer new states of matter to advance fundamental and applied sciences.

Ψk-2015 aimed to foster scientific exchange and outreach. With more than 1200 participants, it was a key event in the field, offering an intensive but enjoyable atmosphere in addition to a chance to explore the coastal city of San Sebastian.

Plenary Speakers
Giulia Galli (U. Chicago)
Georg Kresse (U. Vienna)
Steve Louie (UC Berkeley)
Ingrid Mertig (Martin Luther U., Halle)
Jörg Neugebauer (Max Planck, Düsseldorf)

30 Symposia with 160 Invited Speakers

Thirty Years of Car-Parrinello
Organized by Giulia Galli
Wanda Andreoni (EPFL, Lausanne), Christian Carbogno (Fritz Haber, Berlin),
Michele Ceriotti (EPFL, Lausanne), Robert DiStasio (Princeton U.), François Gygi (UC Davis),
Jürg Hutter (U. Zurich), Heather Kulik (MIT, Cambridge), Angelos Michelides
(London Centre for Nanotechnology), Minoru Otani (U. Tokyo), Annabella Selloni (Princeton U.)

GW and BSE
Organized by Rex Godby and Lucia Reining
Silke Biermann (CPhT, Palaiseau), Antonnio Sanna (Max Planck, Halle),
Francesco Sottile (ETSF, Palaiseau), Mark van Schilfgaarde (King's College, London)

f- electrons: "In memory of Walter Temmerman and his contributions to Psi-k and the electronic structure community"
Organized by Olle Eriksson, O. Andersson, Paul Durham and Silke Biermann
Xi Dai (CAS, Beijing), Nicola Lanata (Rutgers U., Piscataway), Alexander Shick (FZU, Prague),
Julie Staunton (U. Warwick, Coventry), Leonid Pourovskii (CPhT, Palaiseau)

Correlated Electrons
Organized by Markus Aichhorn, Silke Biermann, Massimo Capone, J. Kunes, and Eva Pavarini
Luca de'Medici (ESRF, Paris), Gianluca Giovannetti (SISSA, Trieste), Andy Millis (Columbia U., NY),
Eva Pavarini (FZ, Jülich), Jan Tomczak (TU, Wien); Martin Eckstein (Max Planck, Hamburg),
Philipp Hansmann (CPhT, Palaiseau), Alexey Rubtsov (Moscow State U.), Alessandro Toschi (TU, Wien)

Theoretical Spectroscopy
Organized by Zeila Zanolli and Hubert Ebert
Peter Blaha (TU, Wien), Maurits Haverkort (Max Planck, Dresden),
Jan Minar (LMU, Munich), Patrick Rinke (Aalto U., Esbo)

Recent Advances in Diagrammatic Methods for the Total Energy
Organized by Kristian Thygesen, Patrick Rinke, Georg Kresse and Mark Hybertsen
Garnet Chan (Princeton U.), Andreas Görling (UEN, Erlanger), Fred Manby (U. Bristol),
Thomas Olsen (TU Denmark, Lyngby), Xinguo Ren (UST China, Hefei)

Novel Density Functionals
Organized by Robert Di Stasio, John Dobson and Wanda Andreoni
Florian Eich (UM, Columbia), Paola Gori-Giorgi (VU, Amsterdam),
Per Hyldgaard (Chalmers UT, Göteborg), Karsten Jacobsen (TU Denmark, Lyngby),
Neepa Maitra (Hunter College, New York City), Alexandre Tkatchenko (Fritz Haber, Berlin)

Recent Developments in Density Matrix Functional Theory
Organized by Nicole Helbig and Heiko Appel
Dieter Bauer (Rostock U.), Ralph Gebauer (ICTP, Trieste), Sangeeta Sharma (Max Planck, Halle)

Density-Functional Theory for Coupled Matter-Photon Systems
Organized by Heiko Appel and Michael Ruggenthaler
Heiko Appel (Max Planck, Hamburg) and Michael Ruggentaler (U. Innsbruck),
Kay Dewhurst (Max Planck, Halle), Eberhard Engel (GU Frankfurt),
Ivano Tavernelli (EPFL, Lausanne), Robert van Leuuwen (JYU, Jyväskylä)

Applications of Quantum Monte Carlo Methods
Organized by Matthew Foulkes
Ali Alavi (U. Cambridge), Ethan Brown (RPI, Troy), Ronald Cohen (CIW, Washington, D.C.),
Elif Ertekin (UI, Urbana-Champaign), Leonardo Guidoni (USA, L'Aquila), Sandro Sorella (SISSA, Trieste),
Shiwei Zhang (CWM, Williamsburg), Lucas Wagner (UI Urbana-Champaign)

Upscaling Electronic Structure: Reduced-Scaling and Multi-Scale Methods
Organized by Peter Haynes, Volker Blum, Stefan Goedecker, Javier Junquera, Karsten Reuter, Jorg Neugebauer, Matthias Scheffler and Mike Finnis
Daniel Berger (UC Los Angeles), Luigi Genovese (CEA, Grenoble),
Lin Lin (UC Berkeley), Cedric Weber (King's College, London), Bill Curtin (Brown U., Providence),
Karsten Reuter (TU Munich), Dallas R. Trinkle (UI Urbana-Champaign)

Spin-Orbit Coupling Effects in First-Principles Quantum Transport
Organized by Ingrid Mertig, Paul Kelly, and David Vanderbilt
Frank Freimuth (F. Jülich), Martin Gradhand (U. Bristol), Diemo Koedderitzsch (LMU, Munich),
Qian Niu (UT Austin), Jairo Sinova (JGU, Mainz), Zhe Yuan (JGU, Mainz)

Magnetic excitations and magnetization dynamics
Organized by Ingrid Mertig, Stefan Blugel and Olle Eriksson
Marco Battiato (U. Wien), Hardy Gross (Halle),
Johannes Lischner (UC Berkeley), Samir Lounis (JGU, Mainz)

Chiral Magnetism
Organized by Stefan Blugel
Stefan Heinze (U. Kiel), Yuriy Mokrousov (F. Jülich),
Manuel Pereiro (Uppsala U.), Laszlo Udvardi (Budapest U.)

First-Principles Calculations for Multiferroics and Magnetoelectrics
Organized by Nicola Spaldin and Silvia Picozzi
Eric Bousquet (U. Liege), Lars Nordstrom (Uppsala U.), Massimiliano Stengel (CSIC, Barcelona)

Ab Initio Statistical Mechanics
Organized by Luca Ghiringhelli, Matthias Scheffler and Berand Smit
Tilmann Hickel (Max Planck, Düsseldorf), Roberto Car (Princeton U.), Olle Hellman (Linköping U.),
Alessandro da Vita (King's College, London),Ralf Drautz (RU Bochum), George Booth (U. Cambridge)

Topological Insulators
Organized by David Vanderbilt and Ingrid Mertig
Irene Aguilera (F. Jülich), Liang Fu (MIT, Cambridge),
Kevin Garrity (NIST, Washington, D.C.), Jürgen Henk (F. Jülich)

Electrochemical Energy Storage and Conversion: Solid/Liquid Interfaces
Organized by Marialore Sulpizi, Marie-Pierre Gaigeot and Axel Gross
Kevin Leung (Sandia National Laboratories, Albuquerque), Marie-Liesse Doublet (U. Montpelier),
Adam Foster (Aalto U., Esbo); Axel Gross (Aachen U.), Michiel Sprik (U. Cambridge),
Mira Todorova (Max Planck, Düsseldorf), Enge Wang (CAS, Beijing)

Materials Design
Organized by Nicola Marzari
Thomas Bligaard (Denmark TU, Lyngby), Richard Needs (U. Cambridge), Berend Smit (UC Berkeley),
David Vanderbilt (Rutgers U., Piscataway), Chris Wolverton (Northwestern U., Evanston);
Kristin Persson (Linköping U.), Giovanni Pizzi (EPFL, Lausanne)

Machine Learning Methods in Materials Modeling
Organized by Gabor Csanyi and Alex Tkatchenko
Jörg Behler (RU Bochum), Gabor Csanyi (U. Cambridge), Luca Ghiringhelli (Fritz Haber, Berlin),
Anatole von Lilienfeld (U. Basel)

Hybrid Photovoltaic Materials
Organized by Wanda Andreoni
Filippo de Angelis (U. Perugia), Feliciano Giustino (U. Oxford),
Andrew Rappe (UPenn, Philadelphia), Paolo Umari (U. Padova)

Electron Phonon Coupling and Thermoelectricity
Organized by Christian Carbogno, Nicola Marzari, and Matthieu Verstraete
Lilia Boeri (Max Planck, Graz), Nicola Bonini (King´s College, London),
Claudia Draxl (Humboldt U., Berlin), Gianni Profeta (U. L'Aquila)

Ultrafast Charge Transfer at the Nanoscale
Organized by Stefan Kurth, Robert van Leeuwen, and Gianluca Stefanucci
Oleg Prezdho (U. Rochester), Carlo Rozzi (U. Modena)

Non-Linear Optics of Materials and Nanoplasmonics
Organized by Elisa Molinari, Risto Nieminen, Claudio Attacalite, Myrta Gruning, and V. Venard
Stefano Corni (U. Modena), Pablo García (with FJ García Vidal) (UAM, Madrid), Alberto Castro (FU Berlin),
Stefano Ossicini (U. Modena), Kazuhiro Yabana (U. Tsukuba)

Novel 2D Materials and Heterostructures
Organized by Kristian Thygesen, Stefano Sanvito, Paul Kelly, Nicola Marzari, Adam Kiejna
Geert Brocks (U. Twente), Matteo Calandra (UPMC, Paris), Mei-Yin Chou (GA Tech, Atlanta),
Arkady Krasheninnikov (U. Helsinki), Tony Low (UMN, Minneapolis), Esa Räsänen (Tampere UT)

Modeling of Defect Levels
Organized by Chris van de Walle
Audrius Alkauskas (CPST, Vilnius), Hannu-Pekka Komsa (U. Helsinki),
Sergey Levchenko (Fritz Haber, Berlin), Alfredo Pasquarello (EPFL, Lausanne)

Transport Properties
Organized by Kiyo Terakura, Hardy Gross, and Feng Yuang Ping
Stefan Kurth (UPV/EHU, Donostia/San Sebastián), Jeff Neaton (UC Berkeley),
Giovanni Vignale (UM Columbia), Chun Zhang (NU Singapore)

Matter Under Extreme Conditions
Organized by Hardy Gross and Angel Rubio
Dario Alfe (University College London), Kieron Burke (UC Irvine), Yanming Ma (JLU, Jilin),
and Ronald Redmer (U. Rostock)

Electronic Structure Theory for Biophysics
Organized by Carsten Baldauf, Leonardo Guidoni and Gerrit Groenhof
Carsten Baldauf (Fritz Haber, Berlin), Jochen Blumberger (U. College London), Daniele Bovi (SU Rome),
Ville Kaila (TU Munich), Johannes Neugebauer (WWU, Munster), Ursula Röthlisberger (EPFL, Lausanne)

Special Session: Ψk Volker Heine Young Investigator Award
5 invited talks by the finalists: Andreas Grueneis (Max Planck Stuttgart), Fabio Caruso (University of Oxford)
Ion Errea (UPV/EHU, DIPC), Marco Bernardi (UC Berkeley, LBNL), Johanna Fuks (Hunter College)

JCNS Workshop 2015: Neutron Scattering on Nano-Structured Soft Matter: Synthetic and Bio-Materials

October 5-8, 2015
Tutzing, Germany
http://dipc.ehu.es/ws_presentacion.php?id=122

Organizers
Dieter Richter (Jülich Centre for Neutron Science)
Juan Colmenero (CFM CSIC-UPV/EHU, DIPC)

In the tradition of the annual international JCNS workshops, the Jülich Centre for Neutron Science (JCNS) and the Donostia International Physics Center (DIPC) jointly organized the workshop in 2015.

Neutrons are a key probe providing deep insight into the structure and dynamics and thus in the functioning of synthetic and living soft matter. The workshop discussed the current status, future trends and opportunities of neutron scattering also in combination with simulations.

The topics addressed were:
Functional Polymers
Soft Matter out of Equilibrium
Nano-Composites and Confinement
Nanostructured Complex Fluids
Membranes and Proteins
Soft Matter Materials for Energy Devices

Invited Speakers
Arantxa Arbe (DIPC)
Lise Arleth (University of Copenhagen)
Deborah Berti (University of Florence)
Joao Cabral (Imperial College London)
Stefan Egelhaaf (University of Düsseldorf)
Hitoshi Endo (Japan Atomic Energy Agency)
Henrich Frielinghaus (JCNS)
Thomas Hellweg (University of Bielefeld)
John Katsaras (Oak Ridge National Laboratory)
Tad Koga (Stony Brook University)
Reidar Lund (University of Oslo)
Angel J. Moreno (DIPC)
Kell Mortensen (University of Copenhagen)
Peter Müller-Buschbaum (TUM)
Julian Oberdisse (Université Montpellier 2)
Andrew Parnell (University of Sheffield)
Wolfgang Paul (University of Halle)
Wim Pyckhout-Hintzen (JCNS)
Frank Schreiber (University of Tübingen)
Peter Schurtenberger (Lund University)
Sebastian Seiffert (HZB)
Mitsuhiro Shibayama (University of Tokyo)
Karen Winey (University of Pennsylvania)

21st International Workshop on Inelastic Ion-Surface Collisions (IISC-21)

October 18-23, 2015
Donostia/San Sebastián, Spain
http://iisc21.dipc.org/

Conference Chair
Iñaki Juaristi (CFM CSIC-UPV/EHU, DIPC)

International Scientific Committee
G. Andersson (Flinders University, South Australia, Australia)
F. Aumayr (TU Wien, Inst. of Applied Physics, Austria)
R. Hoekstra (ARCNL, Amsterdam, The Netherlands)
S. Facsko (Helmholtz-Zentrum Dresden-Rossendorf, Germany)
I. Juaristi (University of Basque Country, UPV/EHU,Spain)
K. Kimura (Kyoto University, Japan)
T. Koshikawa (Osaka Electro-Communication University, Japan)
H. Lebius (CIMAP/GANIL, Caen, France)
Ch. Linsmeier (Forschungszentrum Jülich GmbH, Germany)
F. Meyer (Oak Ridge National Laboratory, USA)
J. Pomeroy (NIST, USA)
P. Roncin (ISMO/CNRS, France)
M. Schleberger (University of Duisburg-Essen, Germany)

Local Organizing Committee
Maite Alducin (CFM-CSIC/UPV)
Andrés Arnau (UPV/EHU, DIPC)
María Blanco Rey (UPV/EHU, DIPC)
Ricardo Díez Muiño (DIPC, CFM-CSIC/UPV)
Ivor Lončaric (CFM CSIC/UPV)
Dino Novko (DIPC)

IISC21 was the 21st edition of a series of meetings that started in 1976 in the Bell Labs, Murray Hill, New Jersey, USA. The International Workshop on Inelastic Ion Surface Collisions covered the fundamental aspects of the inelastic interactions of particles with surfaces. It included the following topics:

- Energy loss of particles at surfaces
- Charge exchange between particles and surfaces
- Electron, photon and secondary ion emission due to particle impact on surfaces
- Ion induced desorption, electronic and kinetic sputtering
- Defect formation, surface modification and nanostructuring
- Laser induced desorption. Scattering of atoms, ions, molecules and clusters
- Sputtering, fragmentation, cluster and ion formation in SIMS
- SNMS Cluster/Molecular and highly charged ion beams

Plenary speakers

Gunther Andersson, Flinders University, Australia
Torgny Gustafsson, Rutgers University, USA
Hermann Nienhaus, Universitat Duisburg-Essen, Germany
Thomas Schwarz-Selinger, IPP Garching, Germany
Helmut Winter, Humboldt Universität, Germany

Invited Speakers

Harriet Ahlgren, University of Helsinki, Finland
Frederic Allegrini, Southwest Research Institute, USA
Paola Atkinson, Institut des Nanosciences de Paris, France
Brigitte Ban d'Etat, CIMAP/GANIL, Caen, France
Mark E. Bannister, Oak Ridge National Laboratory, USA
Andrei Borissov, Université de Paris-Sud, France
Peter Bauer, Johannes Kepler Universität, Austria
Bernhard Berger, Technische Universität Wien, Austria
Roman Böttger, Helmholtz-Zentrum Dresden-Rossendorf, Germany
Catia Costa, University of Surrey, UK
Pedro Miguel Echenique Landiribar, Universidad del País Vasco (UPV/EHU), DIPC, Spain
Clara Grygiel, CIMAP/GANIL, Caen, France
Charlotte Herbig, Universität zu Koln, Germany
Hussein Hijazi, Oak Ridge National Laboratory, USA
Maarten van Kampen, ARCNL, The Netherlands
Roland Kozubek, Universitat Duisburg-Essen, Germany
Rafael Martínez Rodríguez, Universidade Federal do Amapa, Brasil
Rosa Monreal, Universidad Autónoma de Madrid, Spain
Kaoru Nakajima, Kyoto University, Japan
Philippe Roncin, Université de Paris-Sud, France
Peter Sigmund, University of Southern Denmark, Denmark
Taku Suzuki, NIMS, Japan
Richard A. Wilhelm, Helmholtz-Zentrum Dresden-Rossendorf, Germany
Yasushi Yamauchi, NIMS, Japan

4th Baskrete Open Days to Industry

November 23-24, 2015
Donostia International Physics Center, Donostia/San Sebastián
http://dipc.ehu.es/ws_presentacion.php?id=125

Organizer
Andres Ayuela (CFM CSIC-UPV/EHU, DIPC)
Jorge S. Dolado (Tecnalia)

The BASKRETE initiative is a collaborative project within the Campus of International Excellence Euskampus carried out between the Basque University (UPV/EHU), the Materials Physics Center (MPC), Donostia International Physics Center (DIPC) and TECNALIA with a twofold mission: On the one hand, BASKRETE will coordinate all the actions which are currently underway in the Basque Country in the field of nanoscience and nanotechnology for cementitious materials. On the other hand, BASKRETE aims to trigger the transfer of high technology knowledge to companies through the establishment of a cooperative program with the industrial agents.

Program

Welcome (P.M. Echenique UPV/EHU, DIPC and R. Díez Muiño, CFM CSIC-UPV/EHU, DIPC)
NanoBasque Initiative (A. Martínez Muro; Nanobasque-SPRI)
BASKRETE initiative (J.S. Dolado, TECNALIA R&I)
An industrial output: NanoSeeds (A. Aramburu, TECNALIA VENTURES)
Dissolution of C3S (H. Manzano, UPV/EHU)
Nanowollastonite formation (J.J Gaitero, TEC)
CSH seeds obtained from by-products (J.S. Dolado, TEC)
A new model of cement Setting (A. Prabhu, TEC)
Ca(OH)2 under pressure (R. Dupuis, DIPC)
Water dynamics in Tobermorite and CSH (S. Cerveny, MPC)
New challenges in valorization of Slag (A. Santamaría, UPV/EHU)

INDUSTRIAL EXAMPLES

Strength retrogression: stability of C2SH (R. Dupuis, DIPC)
Aerogels for Thermal efficiency in Concrete (E. Goiti, TEC)
Synthesis of Superplasticizers (I. Emaldi, POLYMAT)
Anomalous and Normal T11 under pressure (A. Ayuela, DIPC)
C-S-H nanoparticles synthesized by Super Critical Fluid Technology (M. Diez, UPV/EHU and University of Bordeaux)

Euskampus-Bordeaux Symposium

November 26-27, 2015
Donostia/San Sebastián
www.ehubaq.eu/symposium2015/home

This was the second symposium co-organized by the University of Bordeaux and the Euskampus Aggregation (University of the Basque Country, Tecnalia and Donostia International Physics Center (DIPC) within the framework of the Bordeaux-Euskampus Euro-regional Campus of International Excellence.

The Bordeaux-Euskampus Symposium is an event which contributes to structuring and consolidating collaboration between the two academic and university communities, as well as with social stakeholders and organisations whose projects and activities are a key part of the knowledge triangle in the Euro-region of Aquitaine - the Basque Country.

The symposium's program featured 6 types of session or activity:

Plenary sessions: keynote presentation and short presentations on collaborative actions between Bordeaux-Euskampus.

Sessions and activities by and for the community of PhD students: currently in the process of completing a co-supervised or co-tutored thesis: training workshop in transversal competences, poster competition, etc.

Scientific sessions: the aim of these sessions is to establish and consolidate collaborative initiatives focusing on specific themes related to research, value and training. They were designed and coordinated by pairs of researchers from the Bordeaux-Euskampus communities.

Administrative sessions: aimed to structurally facilitate the dynamics of collaboration. They focused on sharing the lessons learned during the experience, as well as on harmonising and improving collaborative procedures between the administrative structures of the two universities.

Quadruple Helix Oriented Sessions: These featured current strategic initiatives to mobilise partners in the Basque Country and Aquitaine. They were made up of representatives of the scientific community, as well as local stakeholders including the authorities, businesses and so on. Their aim was to foster cooperation to elicit local responses to global challenges.

Modelling and Representation. How to make world(s) with symbols

December 10-12, 2015
Donostia International Physics Center, Donostia/San Sebastián
http://www.ehu.eus/en/web/worldmaking2015

Scientific Committee
Catherine Elgin (Harvard)
Paul Humphreys (University of Virginia)
Andoni Ibarra (UPV/EHU)
Thomas Mormann (UPV/EHU)
Hans-Jörg Rheinberger (Max Planck Institute for the History of Science)

Invited Speakers
Catherine Elgin (Harvard)
James Griesemer (UC Davis)
Andoni Ibarra (UPV/EHU)
Tarja Knuuttila (Helsinki Collegium/South Carolina)
Thomas Mormann (UPV/EHU)
Jay Odenbaugh (Lewis & Clark)
Christopher Pincock (Ohio State)
Hans-Jörg Rheinberger (Max Planck Institute for the History of Science)
Iñaki San Pedro (UPV/EHU)
Eric Winsberg (South Florida)

DIPC School

Computation of Electronic Excited States: molecules, aggregates, nanoclusters, nanoparticles, polymers and solids

September 1-4, 2015
Miramar Palace, Donostia/San Sebatián, Spain
http://cees.dipc.org/

Organizers
David Casanova (DIPC, Ikerbasque)
Xabier Lopez (UPV/EHU, DIPC)
Jon Mattin Matxain (UPV/EHU, DIPC)
Mario Piris (UPV/EHU, Ikerbasque)
Fernando Ruiperez (Polymat, UPV/EHU)
Jesus Ugalde (UPV/EHU, DIPC)

The *Computation of Electronic Excited States: molecules, aggregates, nanoclusters,nanoparticles, polymers and solids* international summer school aims to introduce, describe and discuss the theory and applications of computational methods and tools for the study of the electronic structure of excited states in a variety of physical systems: molecules, molecular aggregates, complex systems, nanoclusters and nanoparticles, polymers and solids. The school was taught at the postgraduate level and was especially addressed to PhD students and postdoctoral researchers with a solid background in electronic structure theory and its application within the quantum chemistry and/or physics fields.

The course was divided in two related parts. The first focused on the description of the most relevant and commonly used quantum models for the computational study of electronic transitions. The second part was devoted to the application of the presented methodologies, with specific sessions for different types of systems.

The subjects covered in the school were:
• Electronic structure methods for the study of electronic transitions
• Excited states in molecules
• Excited states in complex systems
• Excited states in extended systems

Invited Speakers

Carlo Adamo (ENSCP-Chimie Paristech, France)
Coen de Graaf (Universitat Rovira i Virgili, Spain)
Andreas Dreuw (University of Heidelberg, Germany)
Johannes Gierschner (IMDEA Nanoscience, Spain)
Anna Krylov (University of Southern California, US)
Stefan Kurth (UPV/EHU, Spain)
Roland Lindh (Uppsala University, Sweden)
Oleg Prezhdo (University of Rochester, US)
Daniel Sanchez-Portal (UPV/EHU and DIPC, Spain)
Carsten A. Ullrich (University of Missouri, US)
Valérie Vallet (CNRS and Universite de Lille, France)
Martijn Zwijnenburg (University College London, UK)

Theses

Theory and simulation of the optical response of novel nanomaterials from visible to terahertz
Mohamed Ameen Poyli
July 2015
Supervisors: Javier Aizpurua and Rubén Esteban

Spectroscopic analysis of atoms and molecules
Alison Crawford Uranga
September 2015
Supervisors: Stefan Kurth and Angel Rubio

Master's Degree Program

UPV/EHU Research Master's in Nanoscience

DIPC 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 Center of Materials Physics (CSIC-UPV/EHU) "Master's in Nanoscience".

The Research Master's in Nanoscience has been offered since 2007. More than eighty students have 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.

Credits

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