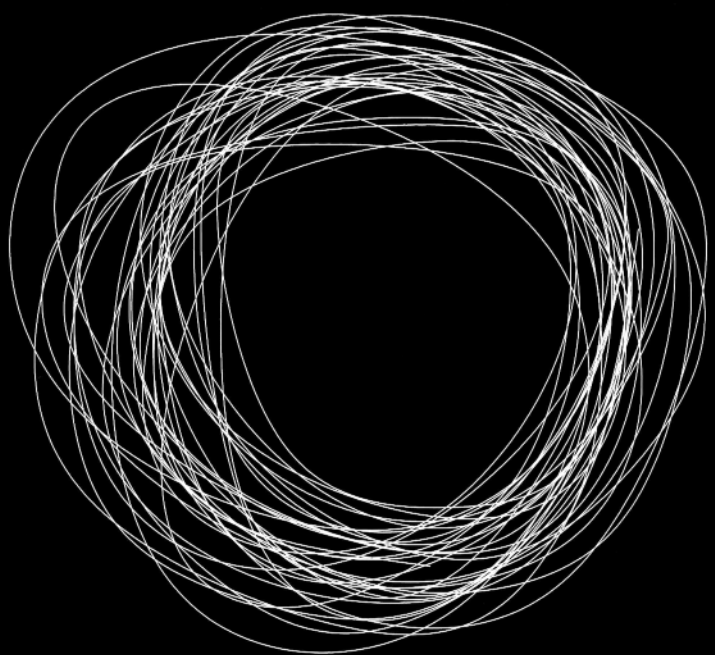
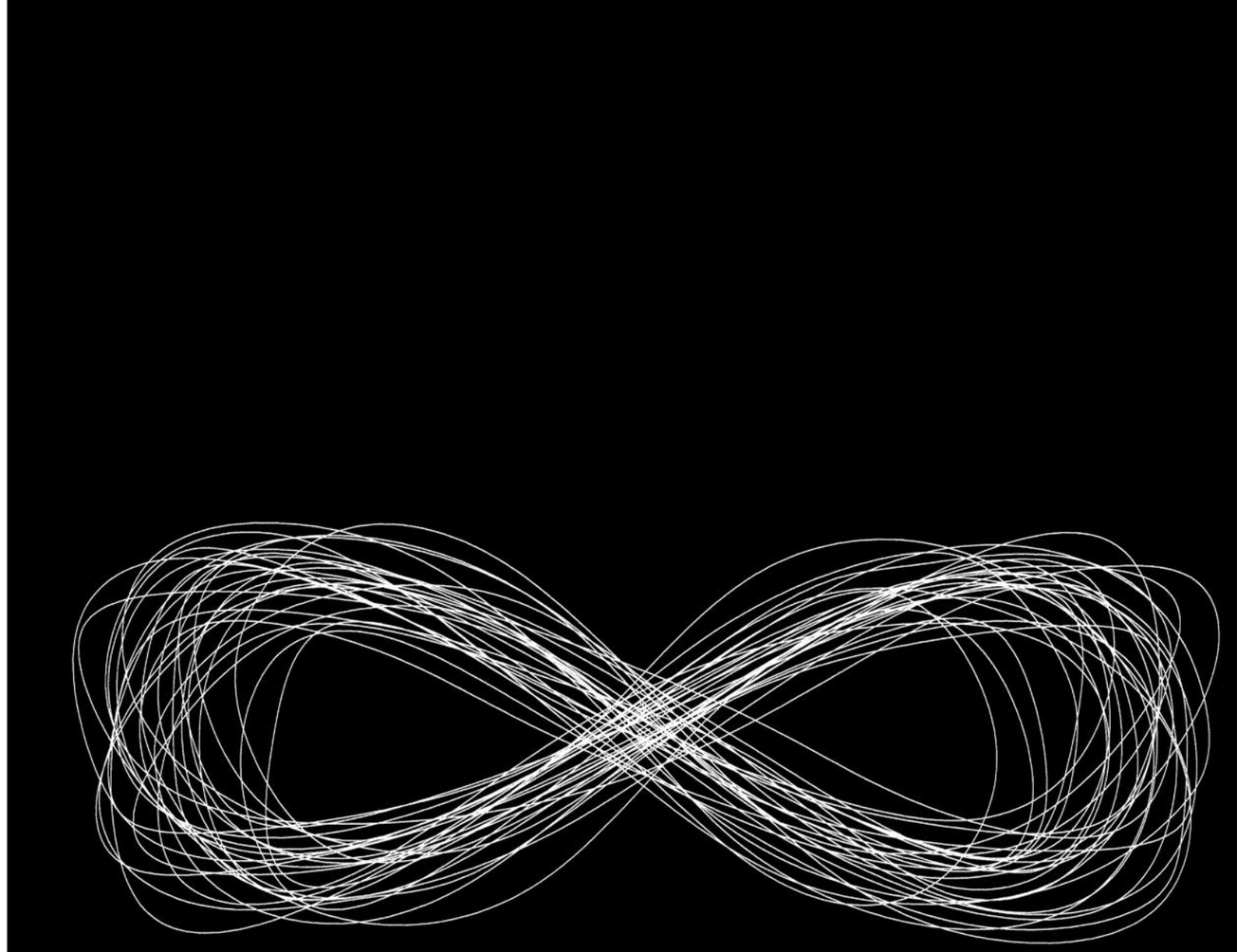
Donostia International Physics Center



Activity Report
12/13

Zero to Infinity by Kit Grover



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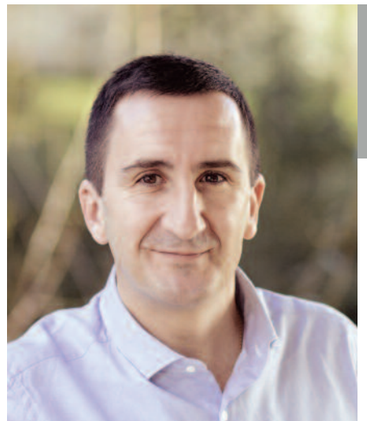
DIPC Activity Report

At DIPC, we do science.



Ricardo Díez Muiño Director

Science is an essential tool of social and economic progress. Advances in scientific research have enormously improved our health and prosperity in the last decades. Testing our life standards against those of just one hundred years ago, we enjoy a longer, fuller, and healthier life in most places on the globe. Distances between different continents seem to have shrunk and we are in close and constant interaction with distant people and remote places. Science has significantly contributed to this new scenario, as well as to the development of modern and sophisticated technologies that are just starting to design our near future.

All this being important, it is no less notable that science has substantially changed our ideas about the world and the way we interact within it. We have reached a deep understanding on tiny particles, immense galaxies, the constituents of matter, and cell function. We are now convinced that our reality can be apprehended and sometimes tuned to cover our necessities. Scientific knowledge has thus become an essential part of our culture and has completely transformed our views on the essence of human nature.

At DIPC we adhere to this spectacular adventure by doing what we know how to do best: scientific research on condensed matter, materials sciences, and nanoscience. DIPC is an open center that gathers local scientists and international visitors because we consider science to be a collective endeavor that always benefits from a diversity of perspectives. DIPC provides a creative and stimulating atmosphere that fosters the exchange of ideas among researchers and thereby the acceleration toward innovative research paths. Scientists at DIPC contribute to the generation of knowledge that can be later applied in new technologies as well as to the training of young researchers that, in the future, can occupy high-profile positions in academia or industry. There is only one indispensable requirement in all DIPC operations: to keep up the high standards of quality that we imposed from the start.

Pedro Miguel Echenique President

When DIPC started in 2000, we could not have anticipated the level of activity that the center was going to achieve. Since then, DIPC researchers have published more than 2,100 scientific articles that have already received about 45,000 citations. Roughly 2,000 scientists have visited DIPC and more than 625 seminars have been scheduled. One of the reasons for this success is that the DIPC structure is very well adapted to ongoing changes in the scientific activity itself: the process of doing science is becoming increasingly collaborative, international, and interconnected. All these features are natural within the DIPC philosophy.

DIPC is devoted to research at the cutting-edge of science, but DIPC also assumes the responsibility of conveying scientific knowledge to society. DIPC feeds an intellectual climate intended to awaken curiosity, interest, fascination and enthusiasm for science and knowledge. In the last years, DIPC has reinforced its Science Communication program and has organized several scientific events that turned out to be extremely gratifying for both scientists and the general public. More than 8,000 people, for instance, attended our Passion for Knowledge Quantum 13 scientific festival that took place in several Basque cities in 2013.

In 2014, DIPC is starting an exciting new program called "DIPC Schools". DIPC Schools are designed to provide young students and researchers with a deeper knowledge on a given research topic in order to improve their research capabilities. They are conceived as intense training sessions lasting from one to two weeks. DIPC Schools will be organized in collaboration with the best Doctoral Schools across Europe, and lecturers will be world-class researchers from the selected fields.

At DIPC, we may feel proud about several things. But there is one thing about which we feel extremely proud: our research team. At DIPC we do a lot of science because our researchers are indeed hooked on science. ■

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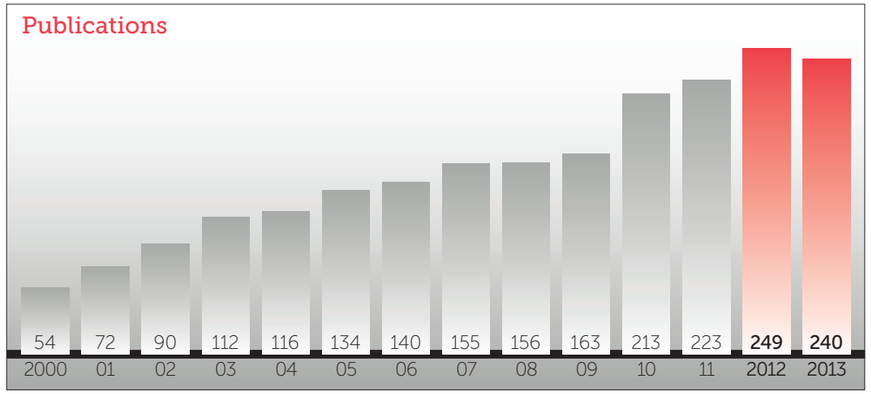
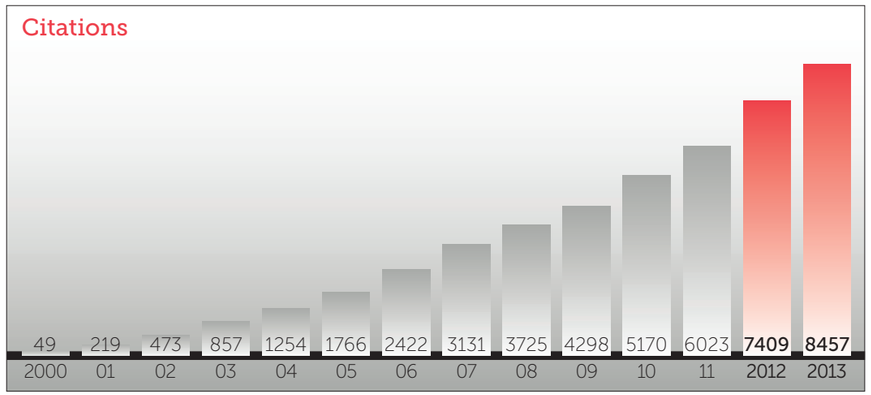


Citations



Scientific Community Events 2012/13

95 Seminars **9** Workshops **2** Courses

Researchers 2012/13

91 Long visits **206** Short visits **7** Theses

Science Communication 12/13

The Science Communication program at DIPC presents science and technology to society. DIPC is a research center dedicated to the advancement of scientific knowledge, but we also assume the responsibility of conveying this knowledge which contributes to progress, culture and freedom.

DIPC proposes meeting spaces for scientists and organizes contact between science and society, cultivating an intellectual climate intended to awaken curiosity, interest, fascination and enthusiasm for knowledge. The Science Communication program seeks to help establish a fluid and permanent dialogue between science and society, and scientists and citizens. Our aim is to foster responsible social and scientific progress in a free and tolerant intellectual environment showing science to be an accessible cultural activity attracting all.

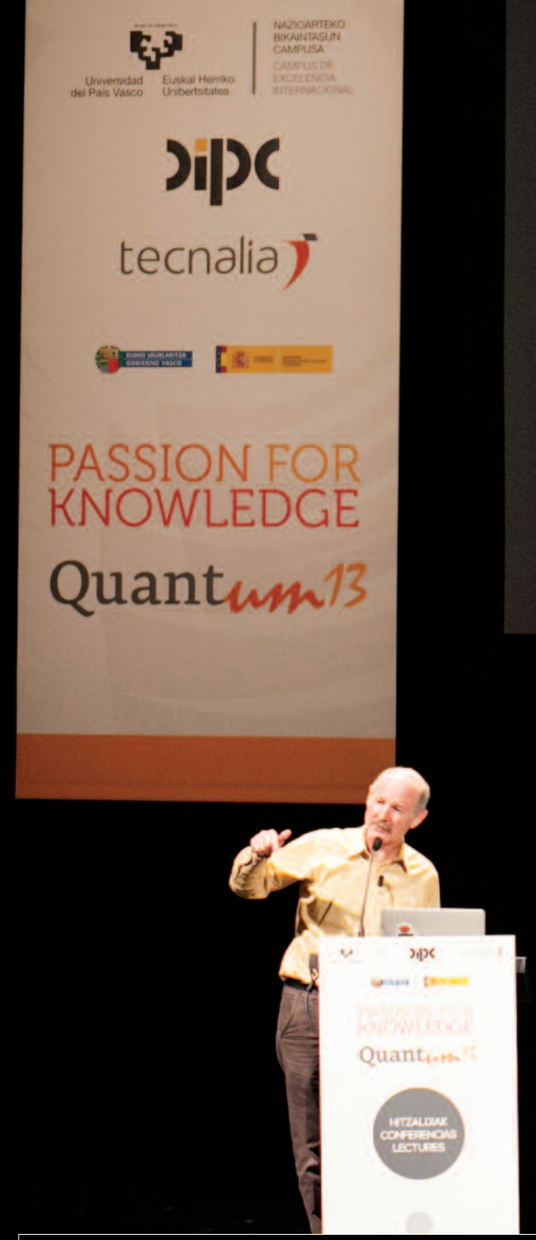
DIPC particularly wishes to cultivate a suitable environment for encouraging young adults to study science and its practical applications, creating a dynamic reserve and channeling the talent of approaching generations.

Science Communication is an ongoing collaboration

Patrons and invited speakers are pictured here at the Victoria Eugenia Theater in Donostia-San Sebastián before the opening of **Passion for Knowledge Quantum 13** on September 30th, 2013. From left to right: Javier Benito, Jon Peli Uriguen, Fernando Cossio, Amand Lucas, Jocelyn Bell Burnell, Claude Cohen-Tannoudji, John Pendry, Iñaki Goirizelaia, Iñigo Urkullu, Pedro Miguel Echenique, Juan Carlos Izagirre, Ignacio Cirac, Cristina Uriarte, Jose Maria Pitarke, Dudley Herschbach, and Rafael Yuste.

As a consequence of the success of Passion for Knowledge in 2010, we organized a new edition, **Passion for Knowledge Quantum 13**, to promote science as a key activity for the well-being of future generations, as well as highlight the thirst of knowledge as the driving force behind scientific, technological and cultural progress. DIPC hosted the event, within the framework of Euskampus, the Campus of International Excellence of the University of the Basque Country (UPV/EHU).

The Keynote Lectures (listed on the next page) gathered 13 prestigious international figures of science, including four Nobel laureates. Topics in the forefront of astrophysics, personalized medicine, neurobiology or genetics were addressed in an event where quantum mechanics became the trending topic. It was an international festival with the 54% of the lectures held in English, 24% in Spanish and 15% in Basque. These Lectures for the general public, held from September 27th to October 1st, attracted more than 4,700 spectators.



www.quantum13.eu

PASSION FOR KNOWLEDGE

Quantum 13 Keynote Lectures

Dudley Herschbach Physical chemistry
Homage to Niels Bohr: Prophet for Paradox

Juan Ignacio Cirac Theoretical physics
The Supercomputers of the Future: What will supercomputers be like in 50 years' time?

José Ignacio Latorre Astrophysics
El Elusivo Boson de Higgs

Aaron Ciechanover Biomedicine
The Personalized Medicine Revolution: Are we going to cure all diseases and at what price?

Rafael Yuste Biology
The Brain Activity Map: Imaging the Activity of Entire Neural Circuits

Dame Jocelyn Bell Burnell Astrophysics
Black Holes in Space

Claude Cohen-Tannoudji Physics
Atoms and Photons: From Optical Pumping to Ultracold Atoms

José María Pitarke Physics
Graphene

Sir John Pendry Photonics
The Science of Invisibility

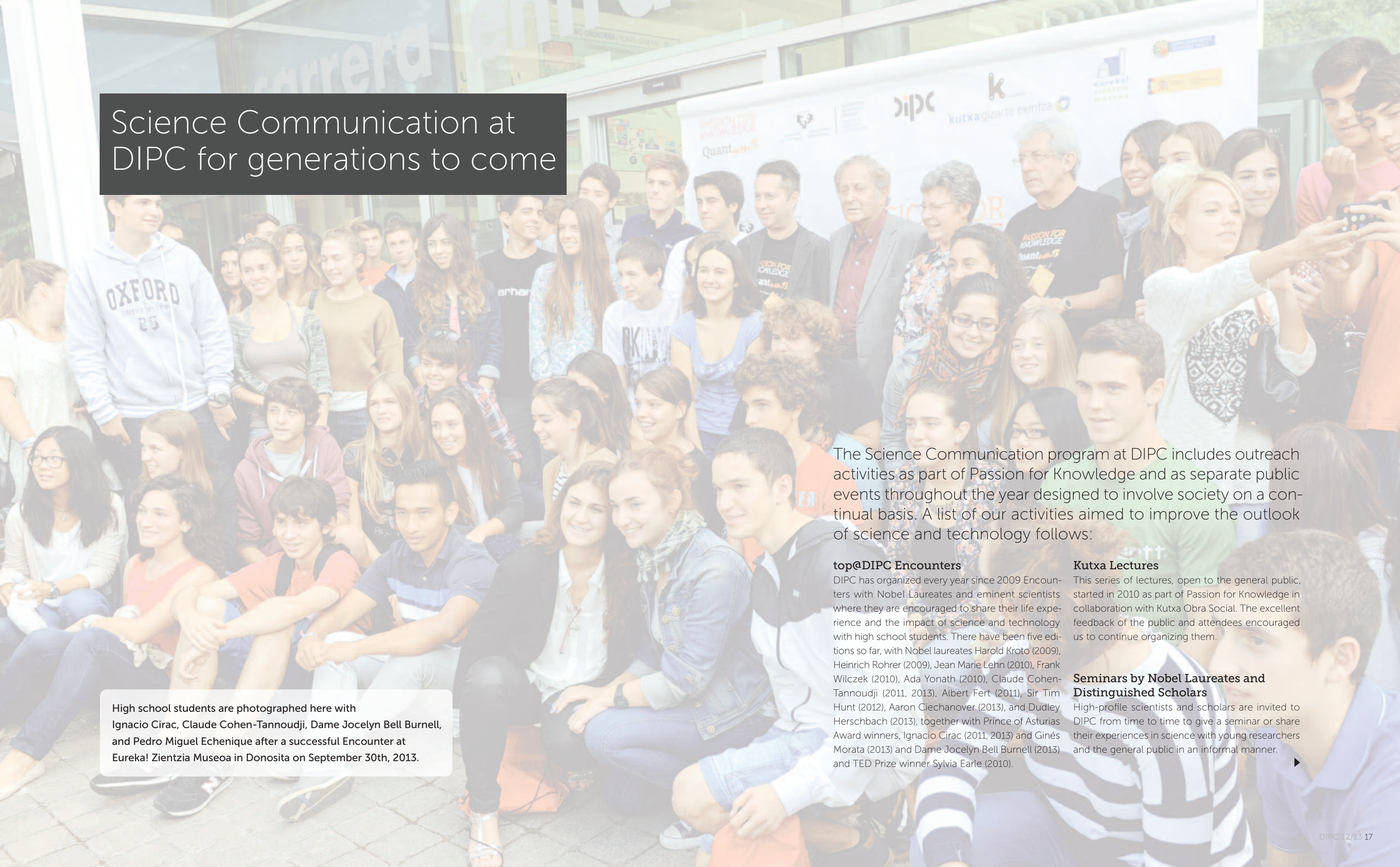
Arantxa Urretabizkaia Literature
We Must Be Doing Something Right in Relation to the Basque Language

Jean-Marie Lehn Supramolecular chemistry
Towards Complex Matter: Chemistry? Chemistry!

Amand Lucas Physics
Niels Bohr, X-Rays and the Secret of Life

Ginés Morata Genetics
Biology in the XXI Century

Science Communication at DIPC for generations to come



High school students are photographed here with Ignacio Cirac, Claude Cohen-Tannoudji, Dame Jocelyn Bell Burnell, and Pedro Miguel Echenique after a successful Encounter at Eureka! Zientzia Museoa in Donosita on September 30th, 2013.

The Science Communication program at DIPC includes outreach activities as part of Passion for Knowledge and as separate public events throughout the year designed to involve society on a continual basis. A list of our activities aimed to improve the outlook of science and technology follows:

top@DIPC Encounters

DIPC has organized every year since 2009 Encounters with Nobel Laureates and eminent scientists where they are encouraged to share their life experience and the impact of science and technology with high school students. There have been five editions so far, with Nobel laureates Harold Kroto (2009), Heinrich Rohrer (2009), Jean Marie Lehn (2010), Frank Wilczek (2010), Ada Yonath (2010), Claude Cohen-Tannoudji (2011, 2013), Albert Fert (2011), Sir Tim Hunt (2012), Aaron Ciechanover (2013), and Dudley Herschbach (2013), together with Prince of Asturias Award winners, Ignacio Cirac (2011, 2013) and Ginés Morata (2013) and Dame Jocelyn Bell Burnell (2013) and TED Prize winner Sylvia Earle (2010).

Kutxa Lectures

This series of lectures, open to the general public, started in 2010 as part of Passion for Knowledge in collaboration with Kutxa Obra Social. The excellent feedback of the public and attendees encouraged us to continue organizing them.

Seminars by Nobel Laureates and Distinguished Scholars

High-profile scientists and scholars are invited to DIPC from time to time to give a seminar or share their experiences in science with young researchers and the general public in an informal manner.

Mestizajes: International Meeting on Literature and Science

Besides traditional ways of reaching understanding, DIPC also explores new and innovative fields of knowledge through its program, "Mestizajes, crossing the boundaries between Art, Science and Humanism". Through the Mestizajes program, a series of workshops and conferences were organized during the last few years where writers, scientists and philosophers have discussed different aspects of the interaction between literature and science. In addition, other projects such as, Writer in Residence and the play "The Interview" have been carried out. Through these activities, the Mestizajes program intends to achieve its main objectives: to explore new forms of knowledge and to make the science closer and more familiar to citizens.

Writer in Residence

This program was launched in 2012 with the aim to explore common spaces between literature and science and boost forms of knowledge based on interaction among people from different spheres. The objectives of the project also include the publication of a scientific work and the creation of a fictional work. Following an international open call, several candidates applied for this program. The winner was writer Eduardo Berti who spent six months at DIPC working in close proximity with scientist, and exploring the common areas of science and literature. As a result, an essay showing common areas between literature and science was co-written by Eduardo Berti and Gustavo A. Schwartz. Eduardo Berti is currently writing a novel based on his experience at the DIPC.

DIPC SPECIAL WEBSITE

dipc.tv

One important landmark in taking science to the general public was the creation of http://dipc.tv in 2008. This web TV serves as a connection platform between DIPC and the general public. The web hosts videos with the different scientific, public and communication activities carried out by DIPC in recent years. Many events, conferences, talks, and activities are streamed live, and others can be downloaded and accessed at the convenience of the users.

SCIENCE VIDEO CONTEST

On Zientzia

Since 2010, a yearly contest to award the best amateur videos created to promote scientific outreach has been organized by DIPC in collaboration with Elhuyar Editorial, and the program Teknopolis from the Basque television (EiTB). The success of the first edition in 2010 with more than 50 videos participating, generated the interest and joy to organize this event again on a yearly basis.

DIPC SPONSORED EVENT

PLAYnano

More than 50 people participated in PLAYnano along with researchers at CIC nanoGUNE. In this game participants discussed the issues posed by the advance of nanotechnology in society and how society should intervene in its development. This initiative is based on the European project PlayDecide.

PUBLIC THEATER

The Interview (La entrevista)

Staged as a meeting between a prestigious scientist at the height of his career and a challenging scientific journalist "The Interview" builds up to a passionate debate about modern-day subjects such as the value and accountability of scientific research and its relation to society and public life. As the plot thickens, the two protagonists cannot avoid revealing a second thread to the story in which both their characters acquire new traits and the relationship between them becomes surprisingly complex. The relationship which is gradually unravelled in "The Interview" and which is based upon personal and moral aspirations and conflicts, clearly conjures up the one between two of the most relevant scientists of the 20th century: the Danish, Niels Bohr and the German, Werner Heisenberg — a relationship which ended abruptly after their famous conversation in Copenhagen in 1941.

SCIENCE BLOG

Naukas Quantum

In collaboration with naukas.com, the popular science blog, a space of short and entertaining talks of 10 minutes, Naukas Quantum, were arranged after the plenary lectures of Passion for Knowledge Quantum 13 on September 1-3 in Donostia-San Sebastián. Well-known collaborators and bloggers of the scientific platform depicted their particular vision of the quantum world and other up-to-date issues.

Passion for Knowledge Quantum 13 Workshops

Valorization of the research and entrepreneurship strategies

Asier Rufino of Tecnalia Ventures covered topics such as: knowledge transfer, patent registry and steps to start-up your company. Nowadays, due to difficulties to get public funding, these points are becoming more important.

Scientific presentation skills

Gonzalo Álvarez, researcher at CSIC and author of El arte de Presentar gave tips to present your scientific results to the scientific community. It was aimed at improving the oral and writing skills of young researchers, especially PhD and Master's students.

How to communicate science to general public

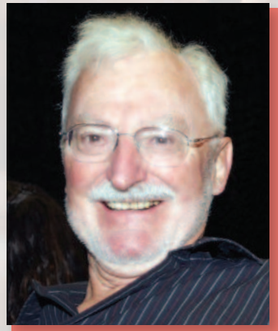
José Ignacio Latorre, professor at the UAB and Cesar Tomé, science popularizer and Mapping Ignorance blog editor, gave their insights about the importance of communicating what they do to general public. Society increasingly demands scientists to explain their work to laymen. This course presented different strategies for how researchers can communicate their work to people in other fields.

Nobel Pitch

This special workshop was based on what is known as the "elevator pitch"; presenting a short, clear and interesting summary of an idea or a project. How would you tell a Nobel laureate about your work in the time that it takes to ride with them in an elevator? Nobel Pitch was aimed at postdoctoral and fellow researchers from different fields of science. They were given the opportunity to meet and interact with Nobel laureates: Aaron Ciechanover, Dudley Herschbach, Claude Cohen-Tannoudji, and Jean-Marie Lehn. Each one was selected to give a pitch on their line of research or project idea in less than five minutes. The session was joined by 70 participants who discussed ideas and general topics with the committee for the advancement of science today after the presentations had been made.

New Ways of Science Lectures

"New ways of science" is a cycle of talks organized jointly by DonostiaKultura and DIPC in an attempt to bring our work closer to society. Scientists from DIPC introduce the fundamentals of Material Science and historical milestones in a clear and attractive way to the general public.



IN MEMORY OF

Heinrich Rohrer (1933-2013)

On May 16th, 2013, Professor Heinrich Rohrer, aged 79, passed away at his home in Wollerau, Switzerland. Together with Gerd Binnig, Heinrich Rohrer designed the first scanning tunneling microscope, a tool that revolutionized the study of atomic-scale systems and opened new avenues in nanoscience and nanotechnology. Rohrer and Binnig received the 1986 Nobel Prize in Physics for this achievement.

In addition to his outstanding talent as a scientist, Prof. Rohrer had an extraordinary talent to motivate fellow scientists, and inspire the general public. An advocate of science as an instrument of progress, he was a relentless communicator of his convictions. Heinrich Rohrer delivered DIPC's opening lecture in 2000 and, since then, we were fortunate to host him as a visiting scientist, as well as benefiting from his contributions at countless science communication events. For DIPC, Heinrich Rohrer was more than a remarkable researcher. He was a compassionate human being and remains an example to us all.

Scientific Highlights 12/13

Charge transport in azobenzene-based single-molecule junctions

Y. Kim, A. Garcia-Lekue, D. Sysoiev, T. Frederiksen, U. Groth, E. Scheer
Physical Review Letters 109, 226801 (2012)

Combined experimental and theoretical study of charge transport across azobenzene-based single-molecule junctions unravels the long-standing debate concerning the conductance of the *cis* and *trans* forms of these photo-switchable molecules.

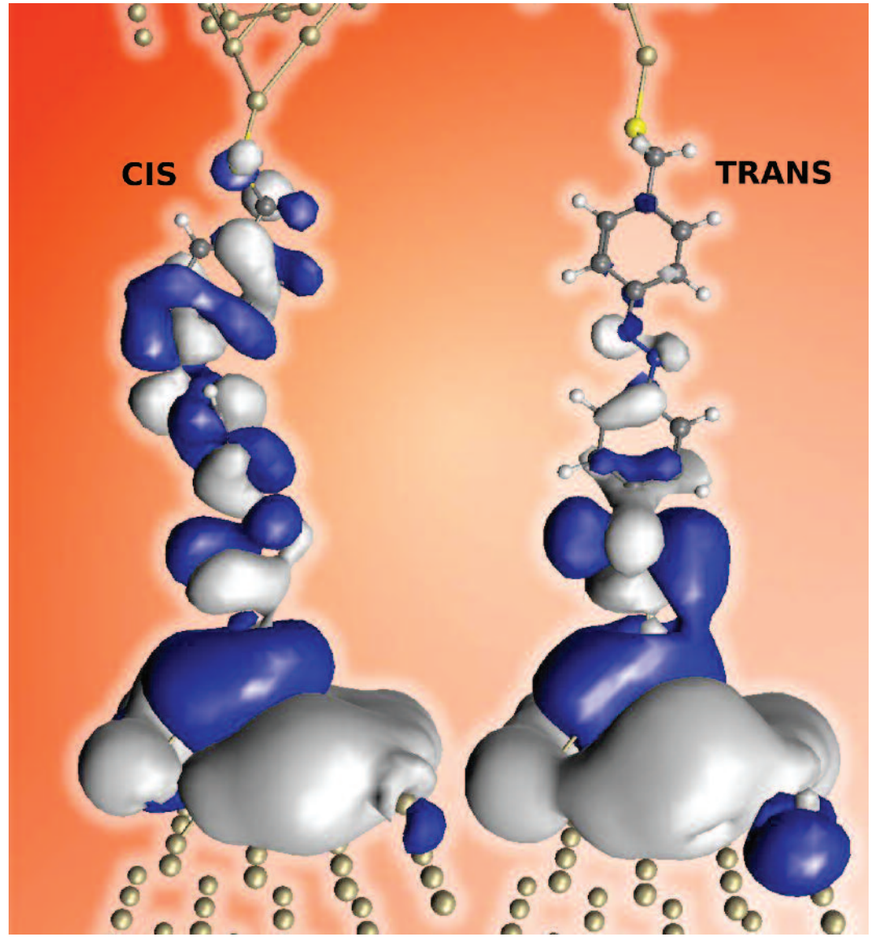
Photochromic molecules are promising building blocks for the realization of functional molecular circuits. In particular, and due to their simple structure, the azobenzene class of molecules has become an archetype of molecular photoswitch research. Azobenzene-derivative molecules change their conformation as a result of a *cis-trans* transition when exposed to ultraviolet or visible light irradiation. Upon this isomerization their electronic properties change markedly, which is expected to induce a significant variation in the conductance of azobenzene-based molecular devices.

Despite the extensive investigations carried out on this type of molecule, a detailed understanding of the charge transport for the two isomers, when embedded in a junction with electrodes, is still lacking. Devices with the *cis* isomer exhibiting either higher or lower conductance than the trans isomer have been reported. In order to clarify this issue, we have performed a combined experimental and theoretical analysis of electron transport through azobenzene-derivative single-molecule break junctions with Au electrodes. Current-voltage and inelastic electron tunneling spectroscopy (IETS) measurements performed at 4.2 K are interpreted based on first-principles calculations of electron transmission and IETS spectra.

Using current-voltage characteristics, we find that the difference in conductance between both isomers is fully caused by a shift of the resonant states. This is confirmed by density functional theory (DFT) based transport simulations, which indicate that the conductance for the *cis* isomer is higher than the *trans* isomer because the current-carrying molecular state is closer to the Fermi energy. It is thus the first study in which it is shown that the *cis* conformation has higher conductance not only because it is shorter, but because the electronic structure of the junction is more suitable to conduct.

In addition, we report for the first time the experimental and theoretical inelastic electron tunneling spectroscopy (IETS) of the photo-switchable molecule in the two different states (*cis/trans*). We show how these IETS fingerprints allow to unambiguously discriminate between the molecular conformations, which thus enables an alternative readout path for identifying the state of azobenzene-based molecular switches.

Unraveling charge transport properties of azobenzene-derivative molecular junctions.



Dominant transmission eigenchannels, i.e. isosurface of the scattering state incoming from the bottom side, for *cis* (left) and *trans* (right) isomers.

Shifts of the molecular vibration modes: fingerprints of isomer states.

Spin-flip transitions induced by time-dependent electric fields in surfaces with strong spin-orbit interaction

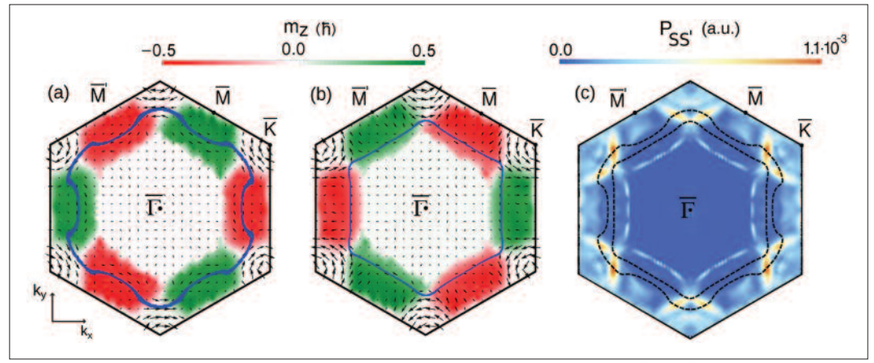
J. Ibañez-Azpiroz, A. Eiguren, E.Ya. Sherman, and A. Bergara
Physical Review Letters 109, 156401 (2012)

Enhanced light induced spin-flip transitions at non-magnetic surfaces with strong spin-orbit coupling, offers an attractive possibility of an experimental approach to the spin-orbit phenomena by optical means.

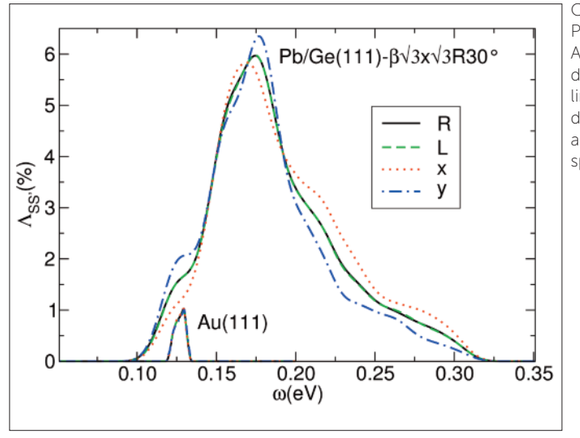
Understanding electron spin transport and spin relaxation in quasi-two-dimensional (2D) systems is of capital importance due to both fundamental reasons and the potential technological applications. The spin-orbit (SO) interaction is the most prominent relativistic effect leading to the fascinating phenomena recently observed in 2D systems, such as the quantum spin Hall effect. An experimentally accessible spin degree of freedom offers a new route for the emergent field of spintronics, where the main features of charge dynamics are strongly influenced by the spin-related effects. The technical possibility of spin manipulation and control by means of an applied bias voltage is strongly supported by recent investigations on a variety of semiconducting alloy samples.

However, a strong SO coupling cannot be achieved in conventional semiconductors, where the spin splitting of conduction electrons is limited to a few meV at most. In contrast, the relativistic effects completely dominate the electronic structure of many heavy-element surface materials and overlayers. The reason lies in the breaking up of the inversion symmetry and the associated gradient of the effective one-electron potential introduced at the interface.

In this article we have presented a comprehensive theoretical investigation of the light absorption rate at a Pb/Ge(111)–β3√×3√R30° surface with strong spin-orbit coupling. Our calculations show that electron spin-flip transitions cause as much as 6% of the total light absorption, representing one order of magnitude enhancement over Rashba-like systems. Thus, we have demonstrated that a substantial part of the light irradiating this nominally nonmagnetic surface is attenuated in spin-flip processes. Remarkably, the spin-flip transition probability is structured in well-defined hot spots within the Brillouin zone, where the electron spin experiences a sudden 90° rotation. This mechanism offers the possibility of an experimental approach to the spin-orbit phenomena by optical means.



(a) and (b) Momentum-dependent spin-polarization structures associated to the S and S' surface states rate at the Pb/Ge(111)–β3√×3√R30° surface, respectively. Arrows represent the in-plane spin polarization component, whereas the background indicates the surface perpendicular component of the magnetization. The Fermi surface of each state is indicated by solid (blue) lines. (c) Spin-flip transition probability associated to the S and S' surface states for R-circularly polarized light. The Fermi surface is indicated by the dashed (black) lines.



Calculated spin-flip absorption rate in Pb/Ge(111)–β3√×3√R30° surface and Au(111). Solid (black), dashed (green), dotted (red) and dashed-dotted (blue) lines represent the results corresponding to the R and L circularly polarized and x and y linearly polarized light, respectively.

Diffusion of hydrogen in Pd assisted by inelastic ballistic hot electrons

M. Blanco-Rey, M. Alducin, J. I. Juaristi and P. L. de Andrés
Physical Review Letters 108, 115902 (2012)

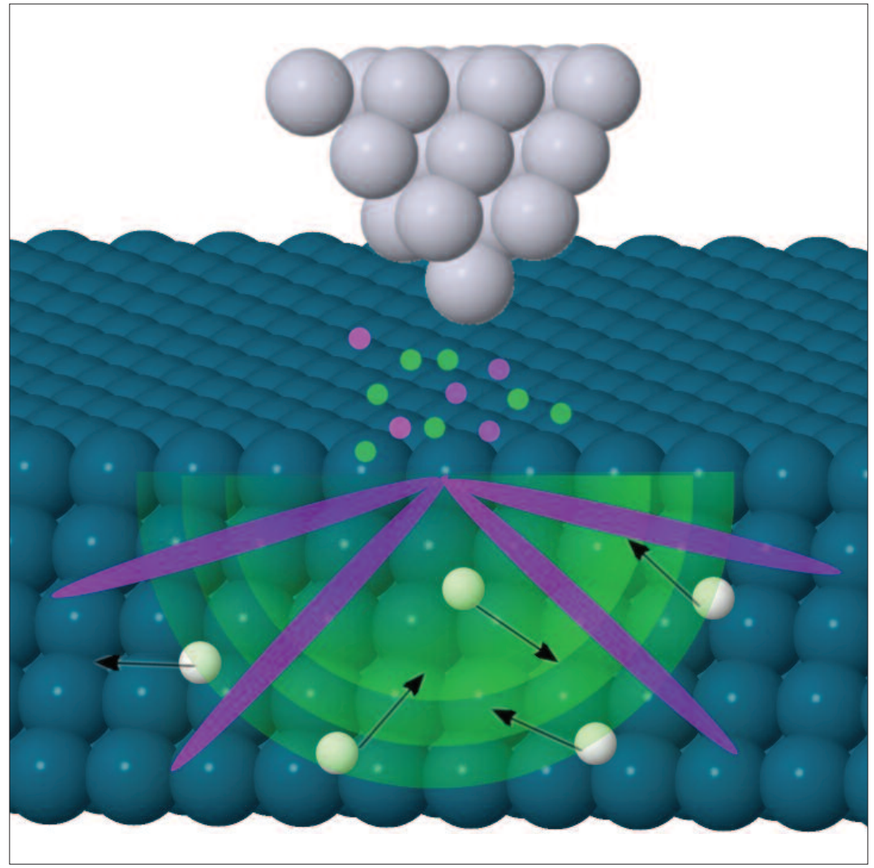
Scanning Tunneling Microscope (STM) has been used recently to manipulate hydrogen atoms deeply buried in a palladium surface. In this paper a model is proposed that explains quantitatively those observations. The usual "on-surface" physics cannot be used in this scenario. Instead, Ballistic Electron Emission Microscopy (BEEM) theory is invoked to describe how carriers propagate layer-wise in the crystal, and to prove that only carriers that propagate freely contribute to the transport of embedded interstitial hydrogen atoms.

An STM tip can be used as a nanoscopic electron gun to promote vibrations in molecules deposited on surfaces or to induce the diffusion of adsorbed atoms. Recently, in an elegant experiment, Sykes et al. made a considerable advance in the field by facilitating atom transport below the surface with a STM tip [Proc. Natl. Acad. Sci. U.S.A. 102, 17907 (2005)]. In particular, they used the tunneling current to extract hydrogen atoms deeply buried below a Pd(111) surface. The nature of the system adds interest because of the applications in hydrogen storage and hydrocarbon synthesis, where subsurface hydrogen can boost the catalytic properties of palladium.

In this paper, scientists from the DIPC put together a theoretical model that accounts for this phenomenon and provides quantitative predictions on the rates at which hydrogen than can be transported under different experimental conditions. The footing of the model is a perturbative description of the coupling between the palladium electronic structure and the hydrogen atom motion. In addition, the model uses imported ideas from the BEEM technique, formerly used mainly to image semiconductor-metal interfaces.

An intriguing experimental finding is that the extraction effect happens with different efficiencies depending on the bias voltage sign, i.e., whether the charge carriers are electrons or holes. This is a central fact that cannot be easily fitted in the well-known palladium electronic structure. The crucial ingredient of the model that reconciles both facts is the distinction between focused and unfocused carriers in the STM current propagating below the surface, as suggested by BEEM theory. Since the former carriers are less likely to interact with the hydrogen atoms, we conclude that the unfocused carriers mainly trigger transport. Focused (unfocused) carriers originate in the d(s)-band of the metal. In particular, we want to draw attention to the fact that the same carrier propagates at the same time according to both s and d-bands of the right energy depending on its momentum, and this is a case where the process of measuring the final state decides whether the carrier stays in a focused or unfocused beam.

This work not only explains a pioneering experiment of manipulation by STM. It also provides a better understanding of the link between BEEM and STM techniques, and how they complement each other. Interestingly, this work has revealed that the current that goes unnoticed during a BEEM experiment is the one that promotes mass transport.



An artist's view of the diffusion mechanism of hydrogen atoms buried in a metal. The tunneling current can be associated to two types of carriers inside the metal: focused and non-focused. The former propagate through narrow channels (magenta), while the latter (green) span larger regions of the metal and are more likely to interact with the embedded interstitial hydrogen atoms.

Contribution from carriers on d-bands is negligible, since they progressively focus along narrow volumes during their layer-to-layer propagation in the crystal.

Ultrafast X-ray pulse characterization at free-electron lasers

I. Grguraš, A.R. Maier, C. Behrens, T. Mazza, T.J. Kelly, P. Radcliffe, S. Düsterer, A.K. Kazansky, N.M. Kabachnik, Th. Tschentscher, J.T. Costello, M. Meyer, M.C. Hoffmann, H. Schlarb and A.L. Cavalieri
Nature Photonics 6, 851-856 (2012)

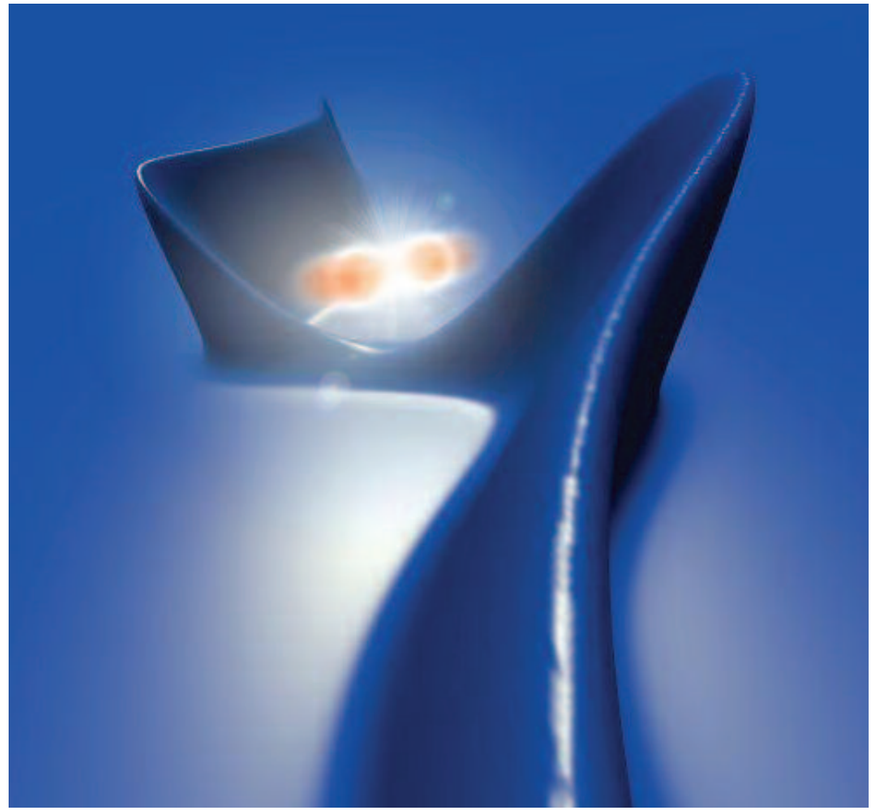
A measurement technique that provides complete temporal characterization of individual FEL (free-electron laser) pulses at DESYs soft-X-ray free-electron laser FLASH.

X-ray pulses delivered by free-electron lasers provide unique research opportunities, because the pulses are ultra-intense and ultra-short. A single FEL pulse lasts for only several tens of femtoseconds, or even less. The FEL X-ray pulses are short enough to study atoms in motion, chemical reactions, and phase transitions in materials with atomic resolution on the femtosecond timescale. However, the precise arrival time and even the temporal profile of the FEL pulse can change dramatically from one pulse to the next. Therefore, to use the FEL to "film" ultrafast dynamical processes, the arrival time of each pulse must be measured to reorder the individual frames or snapshots captured with each individual FEL pulse.

For this measurements a technique used in attosecond science, the "photoelectron streaking", is adapted, so that the temporal profiles of varying light signals can be recorded. For this, the X-ray flashes were shot through neon gas on their way to their target. Each pulse ejects a burst of photoelectrons from the noble gas. The temporal profile of the photoelectrons is a replica of the FEL pulse that ejected them. With an electromagnetic terahertz (THz) field, the photoelectrons are accelerated or decelerated, depending on the exact instant of their ejection. The strength of this effect is measured using time-of-flight spectroscopy. If the exact shape of the terahertz pulse is known, the temporal profile and arrival time of the individual X-ray pulse can be revealed with a precision of about 5 femtoseconds.

The FEL pulse characterization measurements are made without affecting the FEL beam. The technique can be applied in any experiment at almost any wavelength. Until now, no other measurement has provided the complete timing information which is crucial for future application of these unique X-ray light sources. In the immediate future, laser-driven THz streaking will be used to monitor and maintain the FEL pulse duration at FLASH to study a wide variety of atomic, molecular and solid-state systems.

FEL X-ray pulses are short enough to study atoms in motion, chemical reactions, and phase transitions in materials with atomic resolution.



A single-cycle terahertz field accelerates photoelectrons emitted from neon atoms irradiated by an X-ray free-electron laser. In this way, the X-ray pulse temporal profile and arrival time are uniquely retrieved on a pulse-to-pulse basis with femtosecond precision. Credit: Jörg Harms/MPSD at CFEL.

H-atom relay reactions in real space

T. Kumagai, A. Shiotari, H. Okuyama, S. Hatta, T. Aruga, I. Hamada, T. Frederiksen, and H. Ueba
Nature Materials 11, 167 (2012)

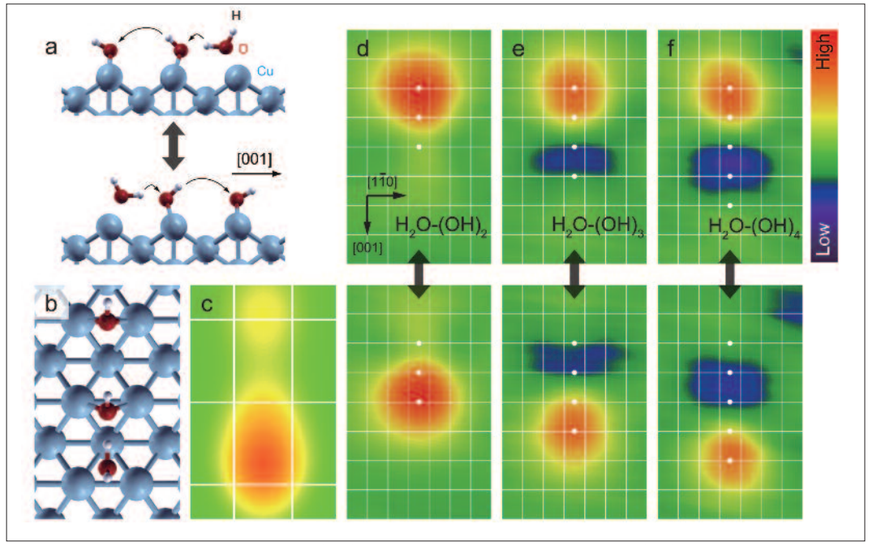
Hydrogen bonds are the path through which protons and hydrogen atoms can be transferred between molecules. The relay mechanism, in which H-atom transfer occurs in a sequential fashion along hydrogen bonds, plays an essential role in many chemical, biological, and materials science processes. In this work the scanning tunnelling microscope was used to construct and operate a test-bed for real-space observation of H-atom relay reactions at a single-molecule level. In combination with ab initio simulations a detailed microscopic picture of the elementary reaction steps was established.

Thanks to a collaboration between scientists at the DIPC and in Japan, a relay reaction of hydrogen atoms has been observed at a single-molecule level using a scanning tunnelling microscope (STM). H-atom/proton dynamics and reactions play crucial roles in, for example, electrode chemistry and heterogeneous catalysis. The relay reaction from one molecular unit to the next is considered to involve coordinated, and often complex, rearrangements within the network, and its study dates back to the idea of 'structural diffusion' introduced by Grotthuss two centuries ago to explain the anomalously high mobility of protons in liquid water. However, a microscopic characterization of relay reactions is extremely challenging in such complex environments.

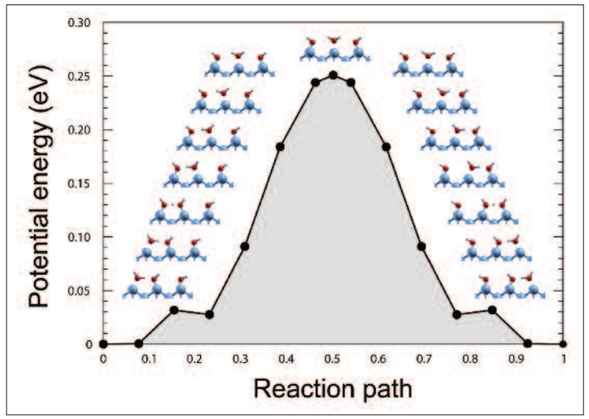
To circumvent this difficulty the researchers engineered a platform of hydrogen-bonded water-hydroxyl chains assembled on a Cu(110) surface in which the H-atom dynamics could be observed at the single-molecule level. By injection of a current pulse through a water molecule at one end of the chain, hydrogen atoms were found to propagate one by one along the chain like dominoes in motion. The reaction turned out to be triggered by excitation of molecular vibrations and to be completely reversible. The experimental findings were rationalized by ab initio calculations for adsorption geometry, active vibrational modes and reaction pathway, to reach a detailed microscopic picture of the elementary processes.

The demonstrated control of H-atom transfer in these hydrogen-bonded molecular chains not only sheds new insight on a fundamental problem. It also opens a new class of single-molecule chemistry with the STM involving hydrogen bonds. Engineering even longer and more sophisticated H-bond systems supported on solid surfaces could provide an opportunity not only to achieve mechanical logic circuits using H-atoms but also to systematically study the fundamental steps of H-atom dynamics in heterogeneous systems. Such systems are conceivable by combining the self-assembling nature of water/hydroxyl complexes with STM manipulation techniques.

The discovery that H-atom transfer along H-bonds is possible directly on metal surfaces further suggests that relay reactions may occur more generally at metal–molecule interfaces and, therefore, in liquids all the way down to the confining surfaces. This is of importance in diverse fields, such as nanofluidics and the design of hybrid materials for proton conduction.



Assembled water-hydroxyl chains on Cu(110) showing H-atom transfer reactions. (a-b) Side and top view of an H_2O–OH–OH chain optimized by DFT calculations and its counterpart. (c) Simulated STM image. (d) Experimental STM images of an H_2O–OH–OH chain and its counterpart superimposed on the lattice of Cu(110) (white lines). The appearance was inverted by a voltage pulse of the STM over the protrusion. The inversion was also observed for (e) H_2O–$(OH)_3$ and (f) H_2O–$(OH)_4$ chains. The dots in (d–f) indicate the nearest short-bridge sites binding oxygen atoms in the chains. The inversion of the appearance corresponds to an H-atom relay reaction in which a sequential H-atom transfer is included, as shown by the curved arrows in (a).



Calculated potential energy surface for the H-atom relay reaction in an H_2O–OH–OH chain on Cu(110) along the [001] direction. The set of images from initial to final states, shown as insets, is computed with the nudged elastic band method. The H-transfer to the center OH is easy (<0.04 eV). The transition state (0.25 eV) corresponds to OH–H_2O–OH with a broken H-bond.

A microscopic picture of the elementary processes was achieved by ab initio calculations.

Do cement nanotubes exist?

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Advanced Materials DOI: 10.1002/adma.201103704 (2012)

Using atomistic simulations, this work indicates that cement nanotubes can exist. The chemically compatible nanotubes are constructed from the two main minerals in ordinary Portland cement pastes, namely calcium hydroxide (CH) and a calcium silicate hydrate (C-S-H) called tobermorite. These results show that such nanotubes are stable and have outstanding mechanical properties, unique characteristics that make them ideally suitable for nanoscale reinforcements of cements.

Researchers at the Donostia International Physics Center (DIPC), Materials Physics Center (CSIC-UPV/EHU), Tecnalia and University of the Basque Country (UPV/EHU) in Spain and at the Technische Universität Dresden in Germany have predicted the stability of cementitious nanotubes. Their new approach may help scientists to synthesize nanotubes made of calcium silicate hydrates, proposed as ideal mechanical reinforcements for cement pastes.

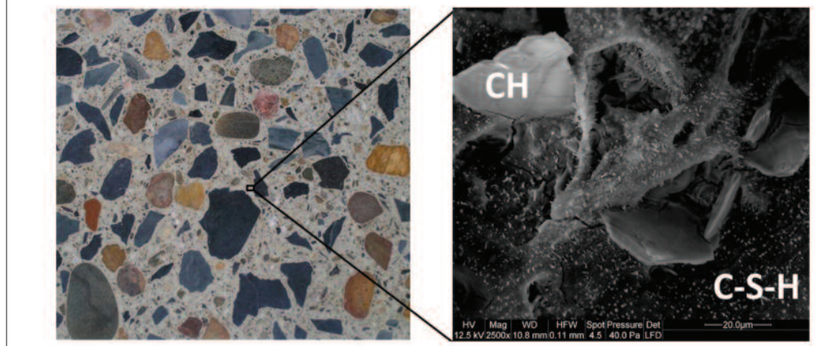
When researchers think of nanoreinforcements, carbon nanotubes come as first option. The problem with carbon nanotubes is that they are water insoluble. In order to make them compatible with water chemistry, they must be functionalized in advance. As a consequence, we thought of directly focusing on inorganic nanotubes, in general, and on cementitious nanotubes, in particular, having a chemistry that is fully compatible with the aqueous solutions of cements.

Previous experiments on nanotube reinforcements of cements haven't fully addressed inorganic nanotubes, which is actually one of our ideas for future development of the field. We are indeed interested in doping cement pastes with already existing inorganic nanotubes, for instance, imogolite ones. By looking at cement microstructure, however, Manzano and co-workers have modelled cementitious nanotubes with the layered structures of portlandite precipitates within the calcium-silicate-hydrate gel. We have predicted that nanotubes made of portlandite Ca(OH)2 are stable and promising candidates to be synthesised as already existing brucite nanotubes Mg(OH)2. Nanotubes built from calcium silicate hydrates themselves are also stable, but their stability is intriguing as it depends on chirality.

The team of researchers showed that especially portlandite nanotubes support strain energies similar to those for already synthesized carbon and inorganic nanotubes. When cementitious nanotubes are synthesized, we proved that they have good elastic properties, with spring constants three times larger than the values of cement gel under compression.

Tensile stresses for cementitious nanotubes also are good for reinforcement. For instance, portlandite nanotubes fail under after a maximum strain of 27% when they reach a maximum stress of about 8 GPa, which is an order of magnitude larger than the stress supported by ordinary steel fibres. Our results strongly suggest that reinforcement at the nanoscale by cementitious nanotubes could even prevent from shrinkage to cement pastes.

Being able to calculate the stability of cementitious nanotubes is very important, as a previous step to their synthesis. Researchers have to see how these nanotubes will be fabricated, but this topic is in the hands of others. The authors in their work just showed the stability and good mechanical properties of these cementitious inorganic nanotubes. They are interested in next describing their survival in different water solutions, where myriad of reactions take place to form the cement paste.



Revealing the quantum regime in tunneling plasmonics

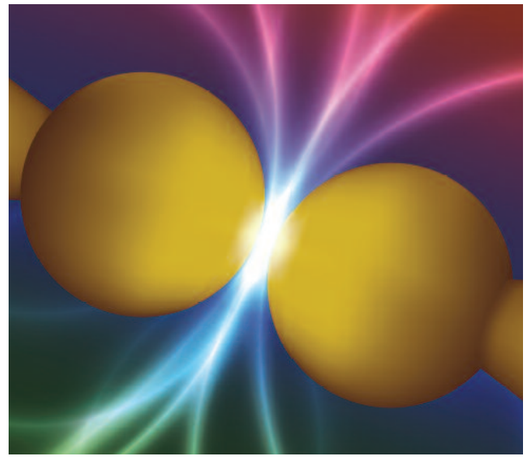
K.J. Savage, M.M. Hawkeye, R. Esteban, A.G. Borisov, J. Aizpurua, and J.J. Baumberg
Nature 491, 574-577 (2012)

The tunneling regime has been observed for the first time by optical methods in the interaction between nano-sized spheres of gold. This quantum regime is identified thanks to the change of colour of the gap or empty space between these particles when they are at distances of less than half a nanometre. This work enables literally "seeing" a quantum kiss between nanoparticles before touching.

The gap generated between two opposing nanospheres of gold can change its colour when the distance between them is less than half a nanometre, according to the investigation by researchers from the DIPC and the CFM (a joint center between the CSIC-UPV/EHU), in collaboration with researchers from the Universities of Cambridge and Paris-Sud. This work enables literally "seeing" quantum mechanics in action and shows how light interacts with matter at subnanometre scales.

To identify the tunneling regime by optical means, tour de force experiments have been combined with very advanced theories. This work, published in Nature, confirms that electrons accumulated on the gold surfaces around the illuminated gap between the two spheres can "jump" from one to the other at optical frequencies, thanks to the tunnel effect, thus reducing the accumulated charge on the surface of each of these spheres and changing the colour of the gap from red to blue, seen as a blueshifting.

When two metallic spheres with a sufficiently small separation between them are illuminated with white light, the gap between them acquires colour thanks to the interaction of the electrons on the surface of the spheres with light. The beam of light 'pushes' the electrons and makes them oscillate. This charge oscillation, a plasmon, gives a red plasmonic colour to the gap. As the spheres get closer, the charge increases which strongly intensifies this red colour. When the distance between both is reduced to under 0.35 nanometres, this accumulation of charge can be seen to drop because electrons can jump across the gap by quantum tunnelling, without the spheres coming into contact with each other. Just as predicted in the quantum theory developed by the research teams in Donostia and Paris, it is possible to identify this quantum electronic jump, because as the accumulated charge drains away, the red colour of the gap changes to blue, that is, a blueshifting of the colour is seen. The change in colour of the gap is the "chromatic fingerprint" that identifies the initiation of the quantum regime therein - an effect that had been predicted by the theoretical team of Nanophotonics at DIPC, and now fully revealed as a result of this research. The reduction in charge at the gap can be allegorically compared with the tension released from a kiss between a romantic couple. As their faces get closer the tension mounts, and only a kiss discharges this energy. In this case, however, the gold nanospheres approaching each other generate a virtual kiss, as they never actually touch, releasing the charge on their surfaces and changing the colour of the gap between them. It is practically like kissing, without the lips actually touching.

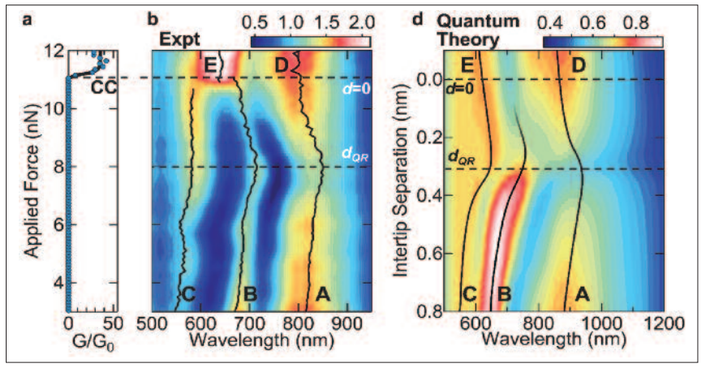


Quantum kisses change the colour of nothing.

Figure showing an arts view of the change of colour as the quantum tunneling effect is triggered out in the subnanometric cavity.

In order to predict the colour changes now confirmed with this experiment, the fusion of the quantum view with the classical view of the world was necessary. Modelling of so many electrons oscillating within the gold particles in response to a beam of light could not be described with existing classical theories therefore new theoretical models needed to be implemented to explain the effect.

This new result establishes a fundamental quantum limit for the minimum dimensions within which light can be trapped. Moreover, this reinterpretation of the interaction between light and matter at the sub-nanometric scale could provide new ways of describing and measuring the atomic-scale world and open doors to novel strategies for engineering even smaller optoelectric technological devices and access new limits of resolution in photochemistry.



Spectral evolution of gap plasmon excitations (A, B and C) when the separation distance of the gap is reduced. At the quantum regime distance (dQR), the modes get screened and blueshift until the full charge transfer modes (E, D) appear when physical contact between the particles is produced. The theoretical model (right hand side) accounts for the main features of the experimental results (left hand side) that classical theories do not reproduce.

Calculating the electronic stopping power from first principles

M.A. Zeb, J. Kohanoff, D. Sanchez-Portal, A. Arnau, J.I. Juaristi, and E. Artacho
Physical Review Letters 108, 225504 (2012)

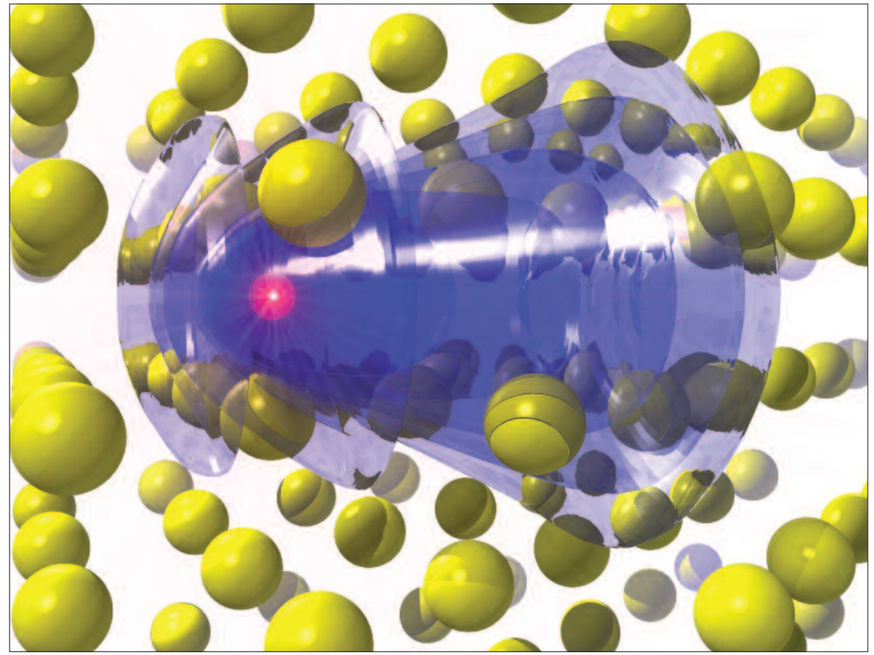
A. Correa, J. Kohanoff, E. Artacho, D. Sanchez-Portal and A. Caro
Physical Review Letters 108, 213201 (2012)

The electronic response to a projectile shooting through a solid can now be quantitatively predicted.

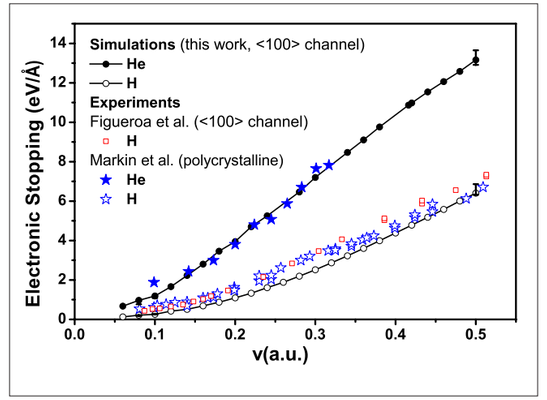
In processes of radiation damage, as encountered in structural materials in nuclear fission or fusion plants, or in materials hosting nuclear waste, or in living tissue under radiation stress, the common culprit is an atomic (or nuclear) projectile traversing matter at high speeds, and producing damage on its passage. Depending on the velocity, many tens of thousands of host atoms can be displaced from their initial configuration in the host material. Part of the damage is by direct transfer of energy from the projectile to the host nuclei, while another part of the projectile's energy transfers to the host electrons.

The latter process is the one dominating at high projectile velocities. It is thus crucial to understand it and to be able to simulate it, if we are interested in simulating the radiation damage processes at all. And we are interested: we need to be able to propose materials for hosting nuclear waste that can withstand damage for a good fraction of a million years. Hardly amenable to direct experimentation. We need accurate predictive simulation techniques to inform that kind of engineering. While there are quite well established first-principles techniques to describe materials for equilibrated electrons, that is not the case for "non-adiabatic processes", that is, for processes in which the projectile moves with a velocity which is comparable or higher than that of the electrons of the host. Although there is qualitative understanding of such processes (the DIPC is a world-wide leading institution in electron stopping of projectiles in metals), the first generic method for the first-principles simulation of such processes was first proposed here in 2007, and has been now proven to be accurate and predictive.

In these two papers (appearing one week apart in Physical Review Letters) electronic excitations in a radiation damage process are accurately described from first principles. In Figure 1 the shape of electronic excitation can be seen when a swift proton moves through bulk aluminium. The rate of energy transfer from the projectile to the electrons (the electronic stopping power) as obtained in the calculations accurately reproduces what obtained experimentally for H and He projectiles in bulk gold (see Figure 2) and aluminium. The calculations use a time-dependent extension of the most standard method for electronic structure prediction, density-functional theory. Once established the predictive power of the method, it is now being applied to situations of interest for the nuclear and space industries.



Isosurfaces (blue) of constant electron displacement density originated by a proton (red) moving in bulk aluminium.



Electronic stopping power for He (upper curve) and H (lower) projectiles in bulk gold as a function of projectile velocity (a.u. stands for atomic units of velocity, 1 a.u. is 0.73 % of the speed of light). Circles with continuous lines are the theoretical results, while the star and square symbols are the experimental values.

The electronic stopping power measures the rate of energy transfer to electrons from an atom moving at high velocity through matter.

Competition between electron and phonon excitations in the scattering of nitrogen atoms and molecules off tungsten and silver metal surfaces

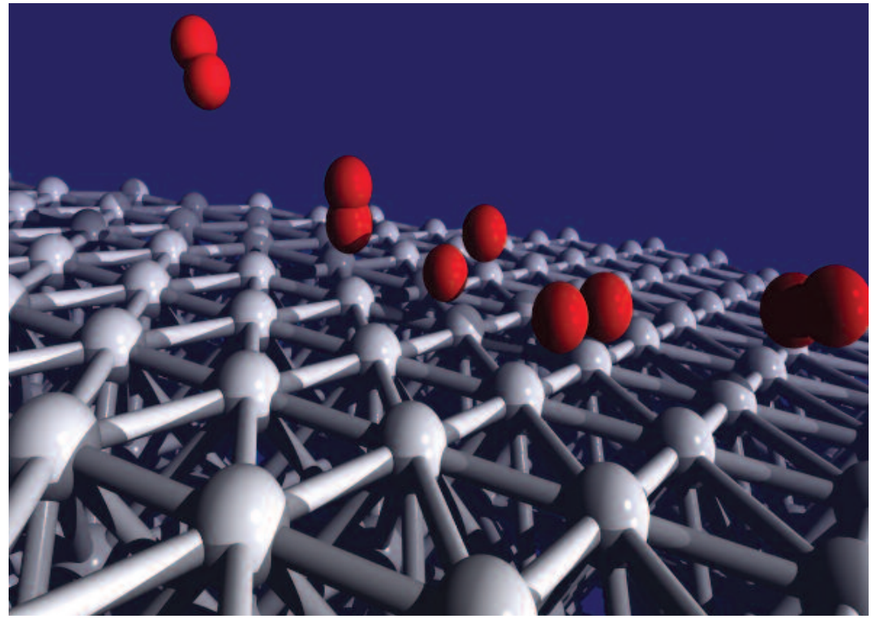
L. Martin-Gondre, M. Alducin, G. A. Bocan, R. Díez Muiño, J.I. Juaristi
Physical Review Letters 108, 096101 (2012)

Energy exchange in the interaction of thermal and hyperthermal molecules and atoms with metal surfaces. A model has been developed to describe phonon and electron-hole pair excitations in simulations of gas/surface dynamics.

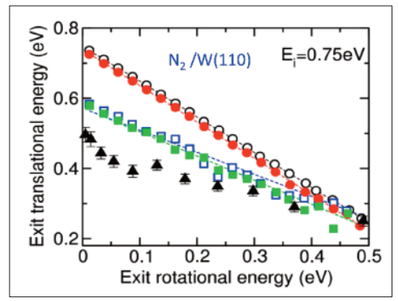
The knowledge of the dynamics of thermal and hyperthermal molecules interacting with metal surfaces has implications in several fields of high technological interest. On the one hand, the industrial production of most of the chemical products implies the use of metallic surface as catalyst. These kinds of chemical reactions need also to be characterized and controlled to limit the erosion of the wall of fusion reactors, or the heating of the surfaces of spacecrafts in their reentry in the Earth atmosphere. For all these reasons, it is very important to be able to simulate the dynamics of gas/surface interactions and reactive processes with the greatest possible accuracy.

The state of the art of the modeling of these processes implies the simulation of the adiabatic dynamics on accurate multidimensional potential energy surfaces. However, recent experiments have shown the need to incorporate into these kinds of simulations the description of energy exchange channels such as the excitation of the movement of the atoms constituents of the crystal lattice of the metal (phonons) and the electronic excitations.

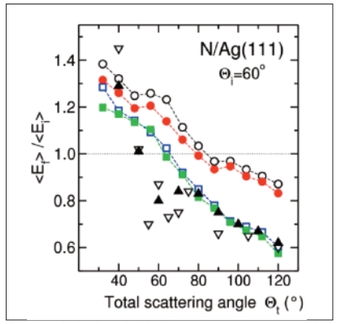
This is precisely what has been achieved in this work. The model presented here has allowed, for the first time, to incorporate the above mentioned inelastic effects keeping the accuracy of the multidimensional potential energy surfaces used in the adiabatic calculations. The model has been applied to the study of two representative systems such as the interaction of nitrogen molecules with tungsten surfaces and nitrogen atoms with silver surfaces. The model has shown its validity by comparison with available experimental results and has been able to explain non trivial effects in the relation between the rotational state and the energy loss of the reflected molecules, and the relation between the energy loss and the exit angle. This work opens new frontiers in the modeling of the elementary reactive processes in the gas/surface interactions and will allow to determine in quantitative terms the relative relevance of different nonadiabatic effects in this kind of problems.



Schematic representation of the dynamics of the interaction of a diatomic molecule with a metal surface.



Exit translational energy of N_2 molecules scattered off W(110) vs the exit rotational energy. Results for normal incidence and detection angles and Ei=0.75 eV initial energy are shown. Our simulations are represented by red filled circles (electron-hole pair excitations), blue open squares (phonon excitations), and green filled squares (electron-hole pairs + phonons). Experimental data are shown by triangles.



Ratio of final to initial average energy vs the total scattering angle for N atoms scattered from the Ag(111) surface. The experimental data (open and filled triangles correspond to different runs of the same experiment) are compared with our simulations for an effusive beam shown as open circles (adiabatic), red filled circles (electron-hole pair excitations), blue open squares (phonon excitations) and green filled circles (electron-hole pairs+phonons).

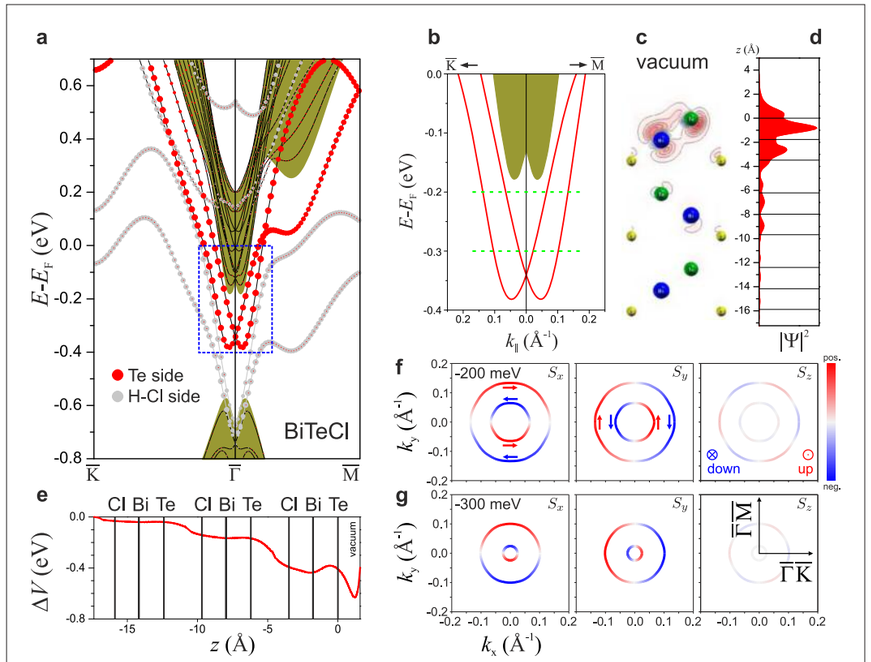
Ideal two-dimensional electron systems with a giant Rashba-type spin splitting in real materials: surfaces of bismuth tellurohalides

S.V. Eremeev, I.A. Nechaev, Yu.M. Koroteev, P.M. Echenique, and E.V. Chulkov
Physical Review Letters 108, 246802 (2012)

Spintronics is aimed at controlling and manipulating the spin degrees of freedom in semiconductor devices. A promising way to achieve this goal is to make use of the tunable Bychkov-Rashba effect that relies on the spin-orbit interaction in a two-dimensional electron system immersed in an inversion-asymmetric environment. We report on a giant Rashba-type spin splitting in two-dimensional electron systems that reside at tellurium terminated surfaces of bismuth tellurohalides, in particular of BiTeCl. The giant spin splitting of the surface state band ensures a substantial spin asymmetry of the inelastic mean free path of quasiparticles with different spin orientations.

The spin-orbit interaction (SOI) that causes spin splitting of electron states in inversion-asymmetric systems is expected to be efficiently exploited in spintronics. The key operating characteristic here is the magnitude of the SOI-induced spin splitting characterized by energy of split states ER and the coupling parameter $\alpha_R = 2E_R/k_R$, which measures the strength of the spin splitting. For the conventional narrow-gap semiconductor structures, the parameter α_R is of order of 10^{-1} eVxÅ. Such a small α_R hampers the development of spintronics devices for room-temperature applications since the latter require a significantly greater spin splitting.

Here, using ab initio calculations, we demonstrate that the 2D electron systems formed at the Te-terminated surface of bismuth tellurohalides in electron surface states (SSs), which split off from the bulk conduction band inherit the giant spin splitting and spin structure from the bulk states. These spin-split SSs provide unique quasiparticle properties of the respective 2D systems, which should be an ideal candidate for a very promising material for spintronics applications. In the figure we show the calculated surface electronic structure of the Te-terminated surface of BiTeCl. One can clearly see the surface state at the Brillouin zone center that demonstrates giant spin-orbit splitting.



(a) Band structure of a thick BiTeCl(0001) slab with hydrogen on the Cl-terminated side; the red (dark gray) and light gray bands are states from the Te- and H-terminated side of the slab, respectively. The size of the red (dark gray) and light gray circles denotes weights of the states localized in opposite, Te and H-Cl terminations of the slab, respectively. The projected bulk band structure is shown in olive green (shaded area). (b) A magnified view of electronic structure of Te-terminated BiTeCl(0001) surface in the vicinity of the Brillouin zone center corresponds to dashed frame marked in the panel (a). Spatial distribution of the Rashba-split state charge density (c) and integrated over (x, y) planes (d). The change of the potential in near-surface layers of the crystal with respect to that in central, bulklike layers (e). Spin structure of the Rashba-split states on Te-terminated BiTeCl(0001), as given by spin projections S_x, S_y, and S_z at energies of 200 meV (f) and 300 meV (g).

Direct imaging of covalent bond structure in single-molecule chemical reactions

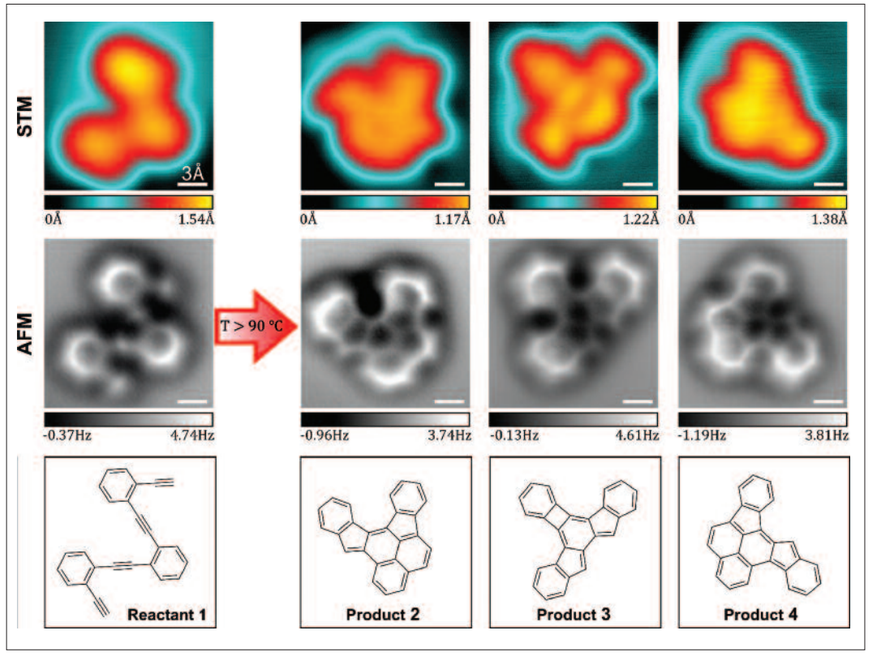
D.G. de Oteyza, P. Gorman, Y.-C. Chen, S. Wickenburg, A. Riss, D.J. Mowbray, G. Etkin, Z. Pedramrazi, H.-Z. Tsai, A. Rubio, M. F. Crommie, F.R. Fischer
Science 340, 1434-1437 (2013)

State-of-the-art non-contact atomic force microscopy is used to provide images of the covalent bond structure of molecular precursors before and after undergoing complex reaction cascades.

The advances of scanning probe microscopy (SPM) have significantly extended the boundaries of molecular imaging. However, even though imaging and manipulation of single atoms in inorganic materials has been routinely performed for many years, comparably high resolution on organic molecules has long remained elusive. Only recently a new benchmark for SPM has been set demonstrating its capability to directly image the chemical structures of organic molecules by tuning-fork-based non-contact atomic force microscopy (nc-AFM). Functionalization of the scanning probe e.g. by individual CO molecules has facilitated superior resolution, rendering images reminiscent of wireframe chemical structures in which even differences in bond-order can be identified. In this present work we use that approach to resolve, for the first time, the structural changes and bond rearrangements associated with complex surface-supported chemical cyclization cascades, an accomplishment currently beyond any other experimental technique. We herein studied the thermally induced enediyne cyclization cascades of 1,2-bis((2-ethynylphenyl) ethynyl)benzene (1). Related precursors have previously been explored for the formation of high molecular weight poly-acenes. However, a variety of competing chemical processes has been shown to play along the traditional Bergman enediyne cyclization. As a consequence, the lack of accurate predictions of the resultant cyclized structures and the complexity of the obtained product distribution exceed the capability of traditional analytical tools to thoroughly characterize the products. We tackle this problem running the reaction under a highly controlled environment on atomically clean Ag(100) surfaces in ultra-high vacuum and by single molecule characterization. This approach has traditionally remained in the realm of scanning tunneling microscopy (STM). However, STM images represent the spatial distribution of molecular orbitals close to EF, additionally broadened and modulated by their hybridization with the electronic states of the substrate (Fig. 1). This leads to a non-trivial contrast in the images that makes the determination of unknown structures a challenging task. Instead, nc-AFM allows direct visualization of the structures of reactant and products (Fig. 1), shedding light onto the transformation reactions. Complementary ab-initio density functional theory calculations further corroborate our experimental results and increase the understanding of the particular reaction pathways.

Hence, in addition to the impact of a direct visualization of chemical reactions, by imaging the complex bond-rearrangements of 1, and complemented with DFT calculations, we provide a detailed mechanistic picture of the cyclization processes previously inaccessible by other experimental tools. In turn, this new insight will guide the design of alternative precursors for the rational synthesis of functional surface-supported molecular architectures.

Visualization of the chemical structures of reactant and products, in combination with DFT calculations, provides invaluable insight into the mechanistic underlying the reactions.



Scanning tunneling microscopy (top row), nc-AFM images (middle row) and wireframe molecular structures of the reactant and the three most common products resulting from annealing the sample to temperatures above 90°C.

We provide direct real space images of the structural changes and bond rearrangements associated with complex surface-supported chemical cyclization cascades, an accomplishment currently beyond any other experimental technique.

Towards tunable charge carrier injection barriers at donor-acceptor/metal interfaces

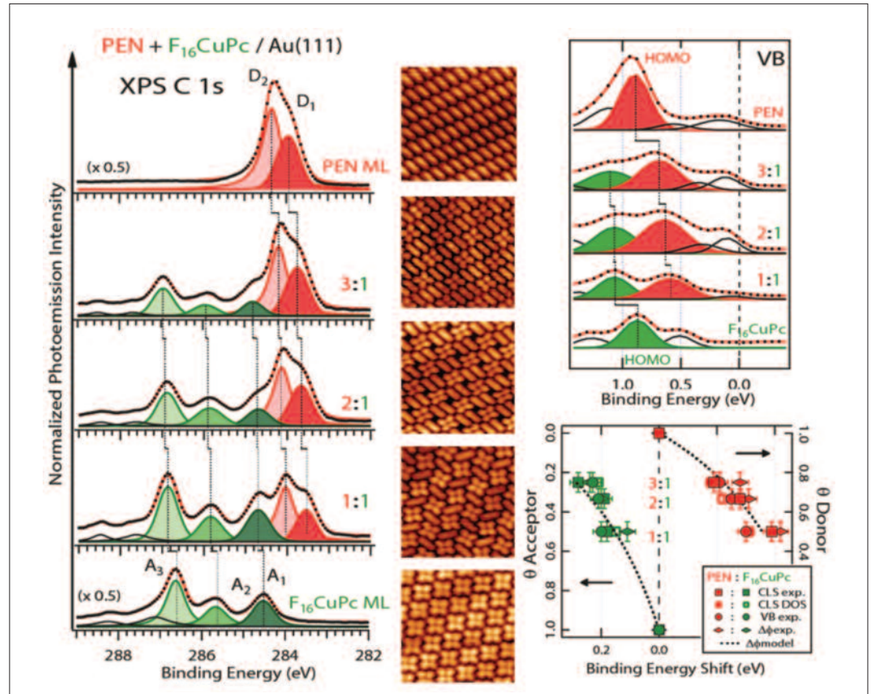
A. El-Sayed, P. Borghetti, E. Goiri, C. Rogero, L. Floreano, G. Lovat,
D. Mobray, J.L. Cabellos, Y. Wakayama, A. Rubio, E. Ortega, D.G. de Oteyza
ACS Nano 7, 6914-6920 (2013)

Experiments on systematically varied donor-acceptor/metal interfaces reveal shifts in the molecular levels that allow tuning charge injection barriers by adjusting the stoichiometry of the blends.

Organic semiconductor-electrode interfaces are among the key elements in charge injection devices and can be generally defined by a monolayer-thick blend of donor and acceptor molecules in contact with a metal surface. Charge injection barriers are determined by the offset from the highest occupied (HOMO) and lowest unoccupied molecular orbital (LUMO) of this contact layer with respect to the Fermi level of the metal electrode. However, the HOMO and LUMO alignment is not easy to elucidate in complex multi-component systems. In addition, it is not well understood how the interface energetics depend on the different supramolecular environments comparing single component layers with molecular blends. Here we demonstrate that core-level photoemission from donor-acceptor/metal interfaces can straightforwardly and transparently assess molecular level alignment. Systematic experiments in a variety of systems show a characteristic binding energy shift in core-levels as a function of molecular donor/acceptor ratio, irrespectively of the molecule or the metal.

In particular, donor levels shift to lower binding energies, whereas acceptor levels shift to higher binding energies. This is exemplified in Figure 1 for the case of pentacene (PEN, donor) and fluorinated copper-phthalocyanines (F16CuPc, acceptor) on Au(111) surfaces. The C 1s core level spectra associated with each of the crystalline structures as a function of molecular stoichiometry are displayed in Fig. 1a, evidencing a rigid shift of all the different components. The same shift is observed in the molecular orbitals, as displayed in Fig. 1b for the respective HOMO levels, and inferred from X-ray absorption spectroscopy (NEXAFS) measurements for the LUMO levels. Interestingly, all these shifts could be reproduced with density functional theory calculations and follow a stoichiometry dependent change in the system's work function (Fig. 1c) in a local vacuum-level pinning scenario. The blend's work function can be further estimated by averaging that of the single component layers, weighted by the partial-coverage of each of the molecules (Fig. 1c).

Our findings therefore demonstrate the possibility to assess interface energetics by core level photoemission, greatly facilitating the characterization of donor-acceptor blends on electrode surfaces. Furthermore, they open a route to tune critical parameters for the efficiency of devices, as are the charge injection barriers at metal-organic interfaces. The interface dipoles associated with donor and acceptor molecules can differ significantly, allowing a substantial range over which to tune the system's work function by the blend stoichiometry in a predictable manner. With this work we therefore don't only advance in the understanding, but also provide a handle for the control of charge injection barriers in technologically relevant donor-acceptor/metal interfaces.



(a) C 1s core-level spectra from donor-rich (top) to acceptor-rich (bottom) monolayer blends, measured by photoemission on the F16CuPc-PEN/Au(111) system at molecular ratios exhibiting long-range crystalline order as previously determined by STM (associated 9.5x9.5 nm2 images on the right). (b) Valence band spectra of the structures shown in (a). (c) Superposition of experimentally measured core-level shifts (filled squares), calculated core-level shifts (empty squares), measured HOMO shifts (filled circles), measured vacuum level shifts (filled diamonds) and vacuum level shifts estimated from single-component data (dotted line), all referred to single component layer values.

The stoichiometry dependent change in the system's work function underlies the observed molecular level shifts.

Direct evidence of two equilibration mechanisms in glassy polymers

D. Cangialosi, V.M. Boucher, A. Alegría, and J. Colmenero
Physical Review Letters 111, 095701 (2013)

Enthalpy recovery over prolonged aging times showed a complex behavior of thermodynamics and dynamics in glassy polymers. The former exhibits two free energy minima in the glassy state. The achievement of each of such minima implies the presence of two equilibration times.

Glassy materials are employed in a wide range of applications and, for this reason, have been deeply investigated along the years. Among them glass forming polymers represent an important class and the study of their molecular dynamics and thermodynamics has been the subject of intense debate. Within this context, most studies have devoted their attention to a temperature range at which the rate of spontaneous fluctuations is shorter than several seconds. This is due to the fact that, in these conditions, equilibrated glasses can be studied over experimental time scales easily accessible in the laboratory practice.

In recent years, experiments in the so-called aging regime as a way to explore the ultraslow molecular dynamics range have been performed. In particular, either the kinetics of recovery of thermodynamic properties or the evolution of the relaxation time during physical aging were monitored on time scales considerably larger than several seconds. Several studies suggest that deviations from the behavior normally observed at relatively high temperatures exist in both the dynamics and the thermodynamics.

In our study, we follow the recovery of equilibrium of the enthalpy of several polymeric glasses previously brought out of equilibrium by cooling them from the equilibrium melt to the glassy state. This is done over prolonged time-scales extending to more than one year. We show that the evolution toward equilibrium of the enthalpy exhibits a two steps recovery. This is shown in Fig. 1 for high molecular polystyrene as a showcase. The first step allows partial recovery of the enthalpy, whereas full recovery occurs after the decay corresponding to the second step. This result demonstrates that the thermodynamics of glasses exhibit two free energy minima. With regard to the dynamics, Fig. 2 shows the temperature dependence of the equilibration times, that is, the time needed to reach each plateau after each step decay. The following scenario emerges analyzing their temperature dependence: i) The equilibration time corresponding to the first step recovery exhibits relatively low activation energy; ii) The equilibration time of the second decay exhibits activation energy similar to that of the polymer segmental relaxation. These results indicate a complex scenario of dynamics and thermodynamics with multiple equilibration steps.

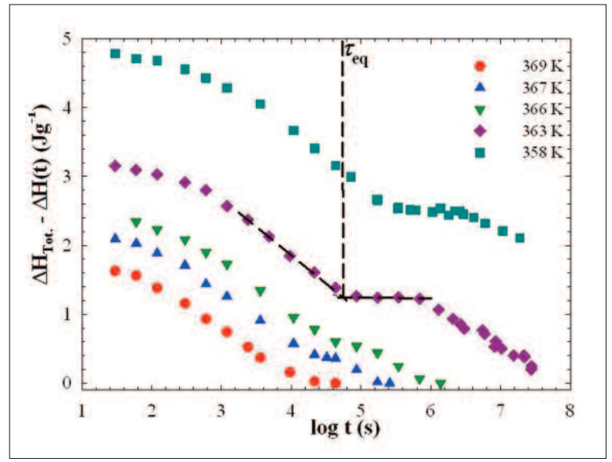


Fig. 1: Time evolution of the recovered enthalpy at the indicated temperatures for high molecular weight polystyrene (PS85k).

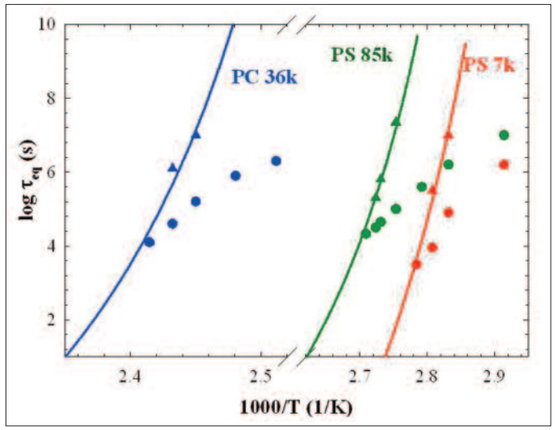


Fig 2: Logarithm of equilibration times corresponding to the first (circles) and the second (triangles) step decay as a function of the inverse temperature obtained from enthalpy recovery data and derived from the temperature dependence of the segmental relaxation (lines).

We show that the evolution toward equilibrium of the enthalpy exhibits a two steps recovery.

Large enhancement of nonlinear optical response in a hybrid nanobiomaterial consisting of bacteriorhodopsin and cadmium telluride quantum dots

A. Rakovich, I. Nabiev, A. Sukhanova, V. Lesnyak, N. Gaponik, Y.P. Rakovich, J.F. Donegan
ACS Nano 7, 2154–2160 (2013)

The development of novel nano-bio hybrid materials that can be integrated into current technologies is one of the most important challenges facing material scientists today. The purpose of this work was to expand research studies in one largely unexplored area of nanobiotechnology: the development of nano-bio hybrid materials that exploit Förster Resonance Energy Transfer (FRET) to enhance the functionalities of technologically-promising photosynthetic biomaterials. One of very promising approaches is to employ semiconductor quantum dots having a broad absorption spectrum as nanoantennae coupled with the natural photosynthetic systems.

Recently it was shown that the nanoscale interactions between semiconductor quantum dots and protein bacteriorhodopsin in the form of Förster resonant energy transfer lead to an improvement of the biological response of bacteriorhodopsin. The reported highly efficient FRET between quantum dots and bacteriorhodopsin indicates that significant improvement of the photoelectric and photochemical properties of bacteriorhodopsin can be achieved.

Furthermore, even more attractive is the possibility to modify the photochromic properties of bacteriorhodopsin, which are inherently connected to the strong nonlinear properties of this protein. The unorthodox idea that FRET-based improvement of the biological response of the bacteriorhodopsin in the presence of quantum dots should influence the nonlinear properties of the bR has not been looked at so far. The feasibility of this approach to develop highly nonlinear nano-bio hybrid structures operating in the FRET regime was in the focus of present work.

Results presented in this paper demonstrated that CdTe quantum dots assembled on the purple membranes containing protein bacteriorhodopsin are able to strongly (up to 4000% at 700 nm) enhance the nonlinear refractive index of bacteriorhodopsin. Using wavelength tunable z-scan technique we find that the enhancement of nonlinear refractive index was significantly smaller at higher wavelengths and only 10-25% in the region of linear absorption (500-650 nm). It is also demonstrated that the bacteriorhodopsin, being a part of an engineered hybrid material, is able to utilize the harvested energy to improve its nonlinear optical properties. Results of this study indicate that both in the linear and the nonlinear regime the quantum dots and the bacteriorhodopsin represent a highly interacting system, and as such, their hybrid material is a good candidate for utilization in device applications.

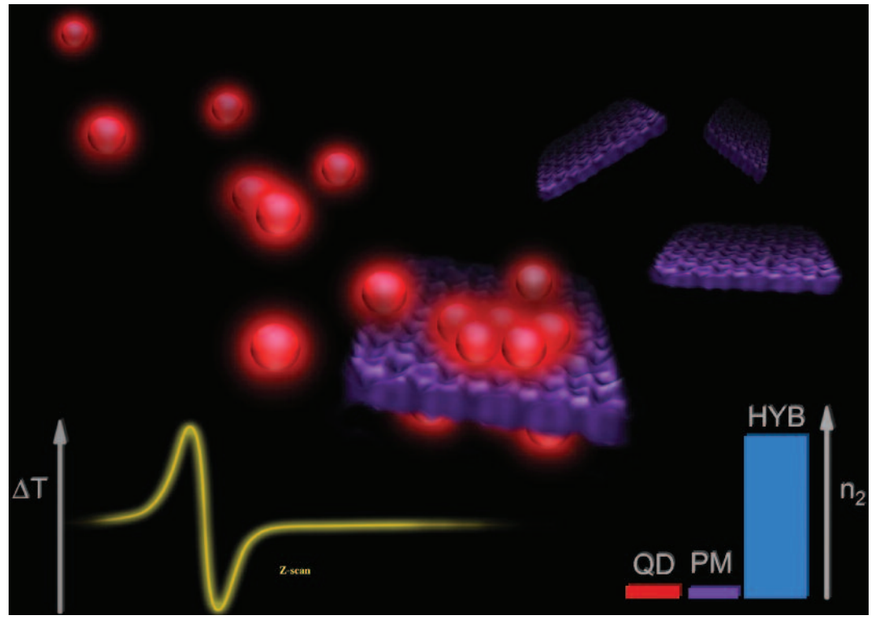
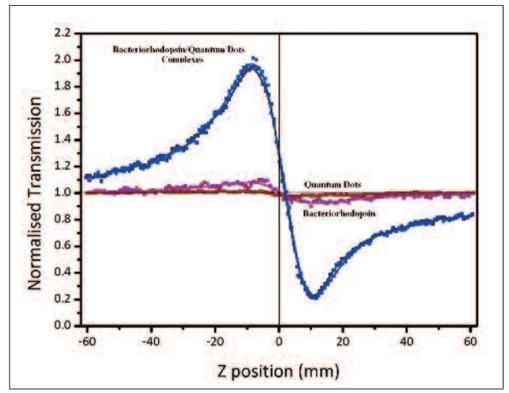


Illustration showing self-assembly of semiconductor quantum dots on membranes containing protein bacteriorhodopsin and typical curve for z-scan nonlinear signal.



Enhancement of nonlinear optical properties in bacteriorhodopsin/quantum dots complexes. Comparison of Z-scan curves for pure bacteriorhodopsin and quantum dots and two bacteriorhodopsin-to-QD complexes.

Quantum dots nano-antennas coupled with the photosynthetic protein bacteriorhodopsin.

Singlet-triplet conversion and the long-range proximity effect in superconductor-ferromagnet structures with generic spin dependent fields

F.S. Bergeret and I.V. Tokatly
Physical Review Letters 110, 117003 (2013)

The long-range proximity effect in superconductor-ferromagnet (S/F) hybrid nanostructures is observed if singlet Cooper pairs from the superconductor are converted into triplet pairs which can diffuse into the ferromagnet over large distances. In this work we have shown that there are other sources of the long-range triplet component (LRTC) of the condensate and established general conditions for their occurrence.

It is by now common knowledge that the interaction between conventional superconductivity and ferromagnetism in S/F hybrids leads to a new type of superconducting correlations in a triplet state. Since the prediction of this intriguing phenomenon in 2001, there has been an increasing experimental activity in the field. That research focuses mainly on the creation and control of superconducting triplet correlations in hybrid structures with the ultimate goal of using polarized spin supercurrents in spintronic devices. To achieve this, it is essential to identify the optimal material combination and hence it is of fundamental interest to understand the physics that underpin triplet generation.

In the present work we have readdressed the problem of singlet-triplet conversion in diffusive S/F structures taking into account the presence of arbitrary (linear in momentum) spin-orbit coupling and go a step further. The main contribution of our work is twofold: First, we have presented a complete analogy between the diffusion of a spin density in a normal metal and the rotation of the triplet condensate in superconducting hybrids. This analogy opens a new view of the singlet-triplet conversion that helps in the understanding of the proximity effect in more complex hybrid structures and suggest the possibility of using the superconducting condensate for encoding spin information.

Second, we have presented for the first time the derivation of the quasiclassical equations for superconductivity in the presence of arbitrary type of SO-coupling. These equations are very useful not only to describe the singlet-triplet conversion but also for the study of the dynamics of S/F hybrids. With the help of these equations we have analyzed different hybrid structures (see Fig. 1) and established the condition for the singlet-triplet-LRTC conversion. For example, according to our work all triplet components can be generated in a S/F/N structure (Fig. 1A), provided the conductor N exhibits a SO coupling. We also have shown that while for a transverse multilayer structure of S/F/S type, the "old" picture of magnetic inhomogeneities can explain the long-range Josephson coupling (Fig. 1C and D), in lateral S/F structures (Fig. 1B), the SO mechanism may be consider as the main mechanism for singlet-triplet conversion. For further reading we also refer to our most recent work: *"Spin-orbit coupling as a source of long-range triplet proximity effect in superconductor-ferromagnet hybrid structures"*, Physical Review B 89, 134517 (2014).

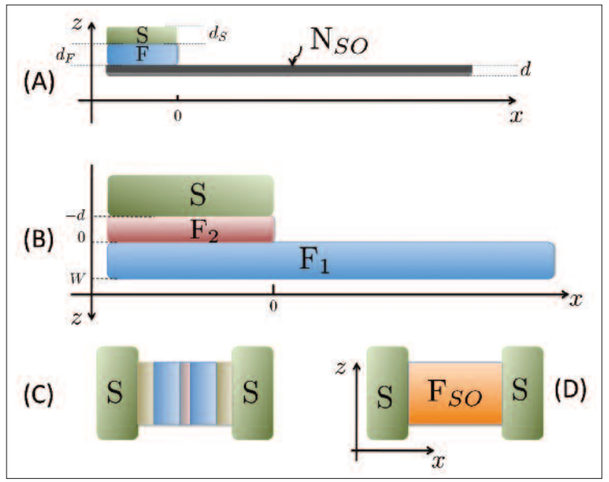


Fig. 1: Different S/F setups for creation of triplet superconducting components: (A) A S/F/NSO structure, with a normal wire with intrinsinc Rashba SO coupling (NSO); (B) a lateral S/F structure consisting of a thin ferromagnetic layer F1, a superconductor electrode and a second ferromagnetic layer, F2 between the S and the F1; (C) and (D) sketched of a transversal multilayer structure commonly used in experiments.

Our work gives a global description of the singlet-triplet conversion in hybrids structures in terms of generic spin-fields and the results are particularly important for the understanding of the physics underlying spintronic devices with superconductors.

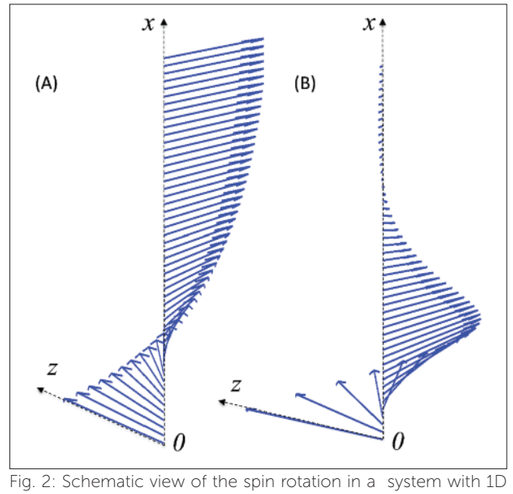


Fig. 2: Schematic view of the spin rotation in a system with 1D inhomogeneity. At $x = 0$ a spin parallel to the *z-axis* is injected. Due to the spin-orbit coupling also the *Sy* component becomes finite upon diffusion. Panel (A) illustrates the spin rotation due to anisotropy of the Dyakonov-Perel tensor, (B) shows the spin rotation due to a fully isotropic spin-orbit coupling. By using our analogy the vectors can also represent the componets of the triplet superconducting correlations upon diffusion into a normal region.

Chemical mapping of a single molecule by plasmon-enhanced Raman scattering

R. Zhang, Y. Zhang, Z.C. Dong, S. Jiang, C. Zhang, L.G. Chen, L. Zhang, Y. Liao, J. Aizpurua,
Y. Luo, J.L. Yang, and J.G. Hou
Nature 598, 82-86 (2013)

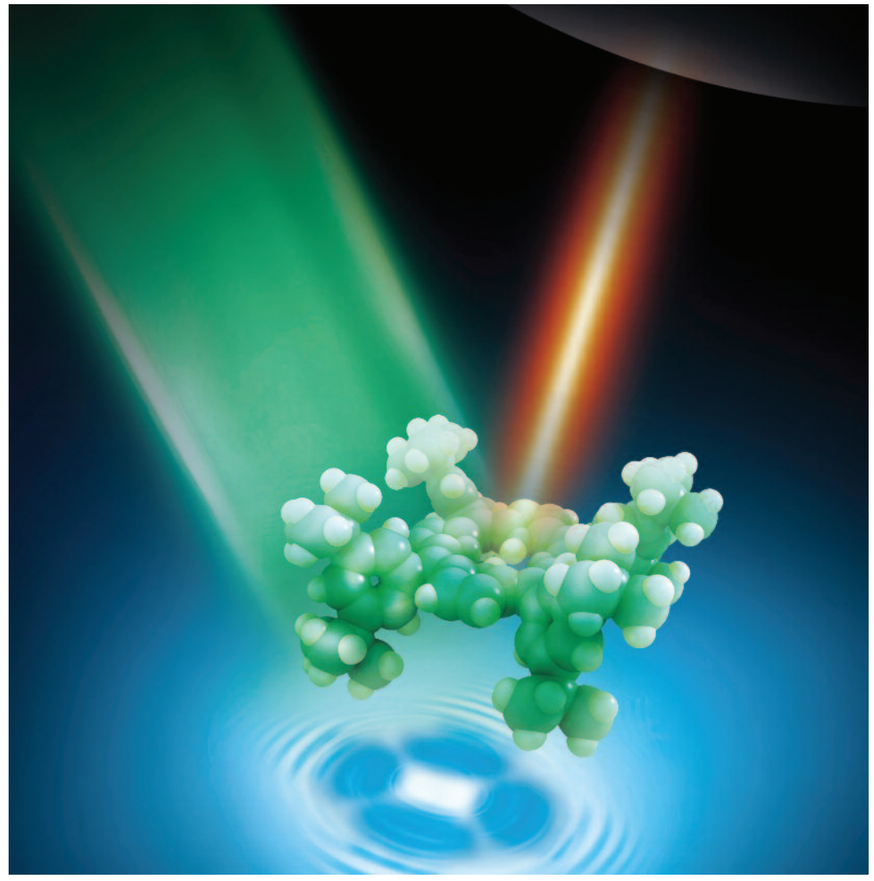
An international team led by Chinese researchers in Hefei (China) with the participation of the Donostia International Physics Center (DIPC) and the Center of Materials Physics (CSIC-University of the Basque Country [UPV/EHU]), has resolved and chemically identified, with a hitherto unprecedented resolution, a single organic molecule using light. This research opens doors to possible technological applications in microscopy, biosensing or quantum information technologies.

Research work led by researchers at the University of Science and Technology of China, in Hefei, in collaboration with the "Theory of Nanophotonics group" at DIPC, have managed to resolve and identify for the first time a single organic molecule with subnanometric-range resolution, using light.

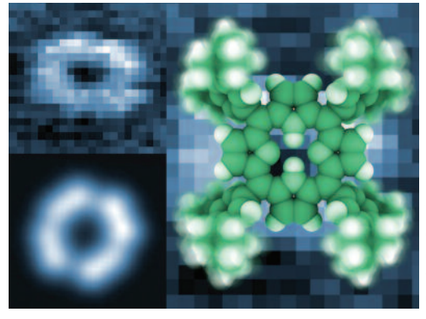
Visible light is an electromagnetic wave whose wavelength is between 400 nanometres (nm), (blue) and 750 nm (red). Due to what is known as the resolution diffraction limit, using light, it is impossible to directly resolve or photograph objects with a size less than half of the wavelength of the light, i.e. less than 200 nm. In order to overcome this limitation, over recent years specialists in Nanophotonics have used metal particles that act as minute optical antennae, concentrating and enhancing the visible light spectrum on a nanometric scale. However, even this technique has its limitations and difficulties when trying to resolve nanometric objects.The optical resolution achieved in this research, hitherto never obtained, has been possible thanks to the combined use of the scanning tunneling microscope (STM) technique in ultra-high vacuum and low temperature conditions, with the Tip-enhanced Raman spectroscopy (TERS) technique, which dramatically enhances the field that acts on the molecule located in the cavity of the tip of the microscope. The combination of these two techniques has enabled "photographing" organic molecules for the first time at a subnanometric scale. The tuning of the collective oscillation of conduction electrons at the tip of the microscope, the so-called plasmons, with the vibrational excitation of the molecule, enables generating a non linear optical signal with sub-nanometric resolution.

When the microscope tip is scanned over the molecule, the Raman signal emitted at each point enables identifying the vibrational signature of the molecule in such a way that, apart from looking "inside" the molecule, it is simultaneously possible to identify which molecule is involved. Researchers at DIPC explain that "it is like peering "inside" the molecule and taking its fingerprints". This level of resolution has only been possible to date using electrons as the probes, but in this research it is the photons of visible light that manage to achieve the miracle of identifying a molecule, going beyond all limits of optical diffraction until now known.

The results of this work open the doors to the direct identification of molecules when their concentration is very small, managing to identify even a single isolated molecule. This ability gives rise to a wide range of possible technological applications, such as in biosensor ones for the analysis of molecular chains, in health and safety for detecting dangerous substances, and in public health for the control of food quality, amongst others. Additionally, accessing to single molecule fingerprints enables the possibility to manipulate and control quantum states of use in quantum information technologies.



Artistic view of a single porphyrin molecule optically mapped by Tip-Enhanced Raman Scattering (TERS), revealing the molecule's vibrational fingerprints with subnanometric resolution (vibrational shadow projected underneath).



Seeing "inside" a single molecule using light.

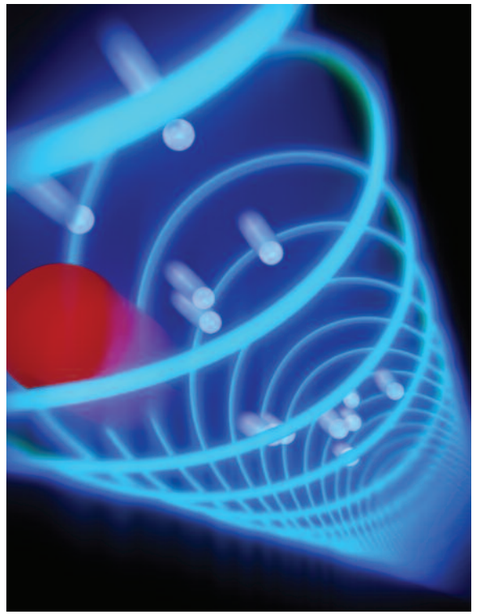
Top left: experimental map of an isolated porphyrin molecule for a given vibration frequency. Bottom left: theoretical calculation of the same molecular vibration showing its fingerprint. Right: molecular structure of the porphyrin used in the experiment.

Optically induced 'negative forces'

A. Dogariu, S. Sukhov and J.J. Sáenz
Nature Photonics 7, 24-27 (2013)

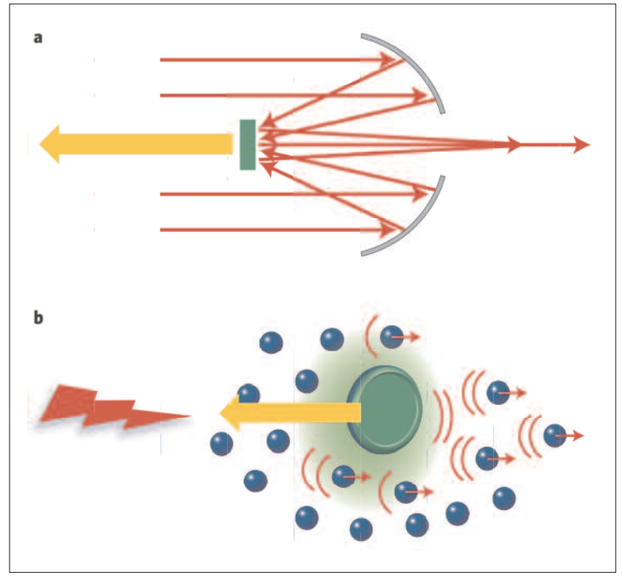
The idea of using optical beams to attract objects has long been a dream of scientists and the public alike. Over the years, a number of proposals have attempted to bring this concept to life. In this work we review the most recent progress in this emerging field, including new concepts for manipulating small objects using optically induced 'negative forces', achieved by tailoring the properties of the electromagnetic field, the environment or the particles themselves.

The potential for light to exert a force along its direction of propagation - a phenomenon known as radiation pressure - is well understood and widely documented. The first indication of this phenomenon came when scientists observed that the tail of a comet always points away from the Sun, regardless of its direction of motion. In the early 1600s, Kepler guessed that the shift of a comet's tail was driven by the pressure of sunlight, and this conjecture still holds true for comet tails that consist primarily of dust. Kepler's belief that the pressure of light is responsible for the solar repulsion of finely divided matter contained in the tail of a comet was accepted and used as an argument for the corpuscular theory by Newton, following which scientists pursued a range of experiments to test the concept of light pressure. On the basis of the newly developed theory of electromagnetism, Maxwell showed that momentum transfer from the electromagnetic field to an object, due to absorption or reflection, should result in a radiation pressure in the propagation direction of the electromagnetic waves.

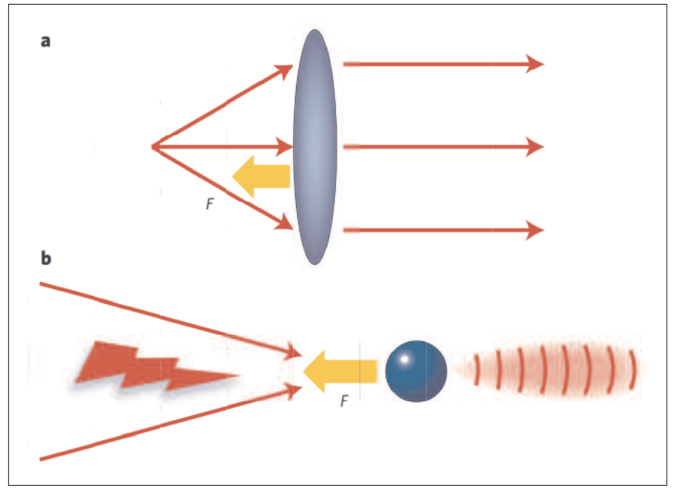


The idea of attracting objects using only the mechanical forces of light is much less trivial. Over the years, scientists have proposed a number of schemes based on employing properties of the electromagnetic field, the surrounding environment, or the particles themselves. These efforts are all fascinating because of their mind-boggling outcome: a seemingly abnormal force that points against the flow of light. In this work we review the main approaches to solving this counterintuitive task and highlight the subtle differences between these endeavours.

The mechanical action of light depends on the structure of the incident electromagnetic fields, the properties of the objects and their surrounding environment.



Pulling forces by tailoring the properties of the object. a) Ordinary optical elements, such as lenses and prisms, can be designed to enhance the forwards scattering such that the electromagnetic momentum of the incident beam is less than that of the emergent beam. b) Analogously, small subwavelength particles can be designed to scatter strongly forwards in such a way that the overall optical force points in a direction opposite to that of the incident beam.



Pulling forces by tailoring the interaction with the environment. a) Conventional telescope. Although the 'total' mechanical action of the light on the system is a pushing force, the effect on the secondary mirror is readily seen to be a pulling force. b) Microscopic equivalent of a). When a plane wave illuminates a set of particles, the total force acting on the system's centre of mass is along the beam. However, it is possible to create a force on some of the particles that acts in a direction opposite to that of the beam propagation.

Quantum chemical study of the reactions between Pd^+/Pt^+ and H_2O/H_2S

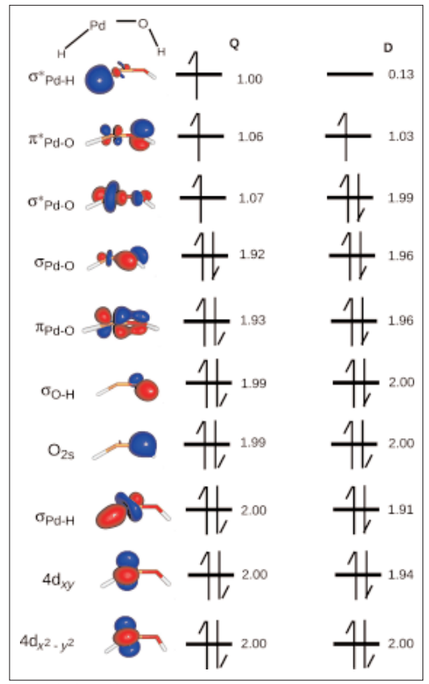
O. Lakuntza, J.M. Matxain, F. Ruipérez, J.M. Ugalde and P.B. Armentrout
Chemistry-A European Journal 19, 8832-8838 (2013)

Although a great deal has been elucidated regarding the mechanism of the reactions between first-row transition-metal cations with water and hydrogen sulfide, much less is known about the reactions of second- and third-row transition-metal cations and of heavier elements as well. Recall that for reactions involving these elements, relativistic effects may play a significant role. Indeed, relativistic effects dominate the chemistry of metal cations with atomic numbers greater than about 50, and the differences in the chemistry of the second- and third-row cations can be largely explained considering the lanthanide contraction. Consequently, it is expected that in the group of nickel, not only for platinum, but also for palladium, the relativistic effects should play an important role in the reactions of these metals or their cations with small molecules. This makes the mechanistic studies of the above mentioned important reactions very challenging, and only affordable at a realistic level by the highest level of theory methods. We have carried out the elucidation of the mechanisims of the reactions between Pd^+/Pt^+ with H_2O and H_2S at such high level of theory.

We propose that the reactions of palladium and platinum cations with water and hydrogen sulfide proceed by the successive migrations of the two hydrogen atoms over the metal center, at which a H-H bond develops to form a complex between the hydrogen molecule and the metal sulfide or metal oxide cation. From these intermediates the loss of H_2 proceeds without a transition state to the corresponding products. Although the energetic parameters depend on the reaction studied, we have found that, whereas both reactions of the palladium occur with two transition states, in the reactions of platinum a third transition state is needed to obtain the final products. In these cases, the second transition state leads to the formation of a dihydrido Kubas-like complex, namely $XPt(H)(H)^+$ (X = O, S) and, through TS3, both hydrogen atoms approach each other, forming the H-H bond.

For all the reactions studied, we have found that one crossing between the doublet and quartet states potential energy surfaces occurs. This spin-crossing takes place around the last transition state, yielding a $H2MX^+$ inter mediate with a quartet ground state.

We have found that the ground state of the $HMXH^+$ intermediate of the four reactions is the doublet spin state, and that the quartet state lies between 1.30 and 1.90 eV above. The study of the molecular orbitals of their corre sponding main valence electronic configurations reveals that, in contrast with the $HNiOH^+$ but along with $HNiSH^+$, they have their doublet and quartet spin states connected by a single electron flip. Furthermore, we have found that, except for the $HPdSH^+$, the energy barrier associated with the $HMXH^+/MXH2^+$ isomerization the is large enough that the $HMXH^+$ should have a long enough lifetime to react with other small molecules like methane.



CASSCF(17,12) natural orbitals and their occupation numbers for the quartet (Q) and doublet (D) states of $HPdOH^+$.

Our calculations predict that only the formation of platinum sulfide is exothermic in both spin states.

Publications 2012

Macromolecular structure and vibrational dynamics of confined poly(ethylene oxide): from subnanometer 2D-intercalation into graphite oxide to surface adsorption onto graphene sheets.
Barroso-Bujans F, Fernandez-Alonso F, Pomposo JA, Cerveny S, Alegria A, and Colmenero J.
ACS Macro Letters 1, 550 (2012).

Probing surface and bulk electrochemical processes on the $LaAlO_3$-$SrTiO_3$ interface.
Kumar A, Arruda TM, Kim Y, Ivanov IN, Jesse S, Bark CW, Bristowe NC, Artacho E, Littlewood PB, Eom CB, Kalinin SV.
ACS NANO 6, 3841 (2012).

Interference, coupling, and nonlinear control of high-order modes in single asymmetric nanoantennas.
Abb M, Wang YD, Albella P, de Groot CH, Aizpurua J, and Muskens OL.
ACS NANO 6, 6462 (2012).

Robust surface doping of Bi_2Se_3 by rubidium intercalation.
Bianchi M, Hatch RC, Li ZS, Hofmann P, Song F, Mi JL, Iversen BB, Abd El-Fattah ZM, Loptien P, Zhou H, Khajetoorians AA, Wiebe J, Wiesendanger R, and Wells JW.
ACS NANO 6, 7009 (2012).

Do cement nanotubes exist?
Manzano H, Enyashin AN, Dolado JS, Ayuela A, Frenzel J, and Seifert G.
Advanced Materials, 24, 3239 (2012).

What Is the maximum coordination number in a planar structure?
Heine T, and Merino G.
Angewandte Chemie-International edition 51, 4275 (2012).

Plasmonics and single-molecule detection in evaporated silver-island films.
Moula G, Rodriguez-Oliveros R, Albella P, Sanchez-Gil JA, and Aroca RF.
Annalen der Physik 524, 697 (2012).

Optical excitation of acoustic surface plasmons in metallic nanoparticles.
Hrton M, Poyli MA, Silkin VM, and Aizpurua J.
Annalen Physik 524, 751 (2012).

Molecular dynamics simulations of iron- and aluminum-loaded serum transferrin: protonation of tyr188 is necessary to prompt metal release.
Mujika JI, Escribano B, Akhmatskaya E, Ugalde JM and Lopez X.
Biochemistry 51, 7017 (2012).

Tunable uptake of poly(ethylene oxide) by graphite-oxide-based materials.
Barroso-Bujans F, Fernandez-Alonso F, Pomposo JA, Enciso E, Fierro JLG, and Colmenero J.
Carbon 50, 5232 (2012).

Easy-dispersible poly(glycidyl phenyl ether)-functionalized graphene sheets obtained by reaction of "living" anionic polymer chains.
Barroso-Bujans F, Boucher VM, Pomposo JA, Buruaga L, Alegria A, and Colmenero J.
Chemical Communications 48, 2618 (2012).

Unexpected trends in halogen-bond based noncovalent adducts.
Huber SM, Jimenez-Izal E, Ugalde JM, and Infante I.
Chemical Communications 48, 7708 (2012).

Planar tetracoordinate carbon in CE_4^{2-} (E = Al–Tl) clusters.
Castro AC, Audiffred M, Mercero JM, Ugalde JM, and Méndez-Rojas MA, and Merino, G.
Chemical Physics Letters 519, 29 (2012).

$sp^{(3)}$ Hybrid orbitals and ionization energies of methane from PNOF5.
Matxain JM, Piris M, Mercero JM, Lopez X, and Ugalde, JM.
Chemical Physics Letters 531, 272 (2012).

Four electrons interacting pairwise in the limit of infinitesimal confining potentials: Especially the quintet spin state.
Akbari A, Amovilli C, March NH, and Rubio A.
Chemical Physics Letters 536, 162 (2012).

Structure and stability of the Si_4Li_n (n = 1-7) binary clusters (vol 522, pg 67, 2012).
Osorio E, Villalobos V, Santos JC, Donald KJ, Merino G, and Tiznado W.
Chemical Physics Letters 539, 252 (2012).

Fermi sea excitations in the optical spectrum of a doped ^{3}He droplet.
Benedek G, and Hizhnyakov V.
Chemical Physics Letters 548, 17 (2012).

Densely substituted unnatural L- and D-prolines as catalysts for highly enantioselective stereodivergent (3+2) cycloadditions and aldol reactions.
Conde E, Bello D, de Cozar A, Sanchez M, Vazquez MA, and Cossio FP.
Chemical Science 3, 1486 (2012).

Supramolecular assembly of diplatinum species through weak Pt(II) Pt(II) intermolecular interactions: a combined experimental and computational study.
Perez Paz A, Espinosa Leal LA, Azani M-R, Guijarro A, Sanz Miguel PJ, Givaja G, Castillo O, Mas-Balleste R, Zamora F, and Rubio A.
Chemistry a European Journal 18, 13787 (2012).

The nature of chemical bonds from PNOF5 calculations.
Matxain JM, Piris M, Uranga J, Lopez X, Merino G, and Ugalde JM.
Chemphyschem : a European journal of chemical physics and physical chemistry 13, 2297 (2012).

Stabilizing H_3^- : or are we stabilizing a proton?
Grabowski SJ, and Hoffmann R.
Chemphyschem:a European journal of chemical physics and physical chemistry 13, 2286 (2012).

Energy dissipation channels in the adsorption of N on Ag(111).
Martin-Gondre L, Bocan GA, Alducin M, Juaristi JI, and Díez Muiño R.
Computational and Theoretical Chemistry 990, 126 (2012).

Classical dynamics study of atomic oxygen over graphite (0001) with new interpolated and analytical potential energy surfaces.
Morón V, Martin-Gondre L, Crespos C, Larregaray P, Gamallo P, and Sayós R.
Computational and Theoretical Chemistry 990, 132 (2012).

Normalization of the Gaussian binning trajectory method for indirect reactions.
Bonnet L, Larregaray P, Arbelo-Gonzalez W, and de Castro-Vitores M.
Computational and Theoretical Chemistry 990, 30 (2012).

Non-covalent interactions in $NH_4^+...(C_2H_2)_n$ ammonium cation-acetylene.
Grabowski SJ.
Computational and Theoretical Chemistry 992, 70 (2012).

Non-covalent interactions preface.
Alkorta I, and Grabowski SJ.
Computational and Theoretical Chemistry 998, 1 (2012).

The strength of frustration and quantum fluctuations in $LiVCuO_4$.
Nishimoto S. Drechsler SL, Kuzian R, Richter J, Malek J, Schmitt M, van den Brink J, and Rosner H.
EPL 98, 37007 (2012).

Editorial: Challenges and solutions in GW calculations for complex systems.
Giustino F, Umari P, and Rubio A.
European Physical Journal B 85, 319 (2012).

Zero point motion effect on the electronic properties of diamond, trans-polyacetylene and polyethylene.
Cannuccia E, and Marini A.
European Physical Journal B 85, 320 (2012).

Electronic and magnetic properties of NiS_2, NiSSe and $NiSe_2$ by a combination of theoretical methods.
Schuster C, Gatti M, and Rubio A.
European Physical Journal B 85, 325 (2012).

Study of tetrabutylammonium bromide in aqueous solution by neutron scattering.
Bhowmik D, Malikova N, Teixeira J, Meriguet G, Bernard O, Turq P, and Haussler W.
European Physical Journal-Special Topics 213, 303 (2012).

Molecular conductance in relation to inverse transport theory and to chemical bond order.
Klein DJ and March NH.
International Journal of Quantum Chemistry 112, 99 (2012).

Ab initio study of 2DEG at the surface of topological insulator Bi_2Te_3.
Vergniory MG, Menshchikova TV, Eremeev SV, and Chulkov EV.
Jetp Letters 95, 213 (2012).

Giant Rashba-type spin splitting at polar surfaces of BiTeI.
Eremeev SV, Nechaev IA, and Chulkov EV.
Jetp Letters 96, 437 (2012).

Natural sulfur-containing minerals as topological insulators with a wide band gap.
Silkin IV, Menshchikova TV, Otrokov MM, Eremeev SV, Koroteev YM, Vergniory MG, Kuznetsov VM, and Chulkov EV.
Jetp Letters 96, 322 (2012).

Effects of the electron-electron interaction on the surface of three-dimensional topological insulators.
Nechaev IA, and Chulkov, EV.
Jetp Letters 96, 480 (2012).

Isotope effect in the superconducting high-pressure simple cubic phase of calcium from first principles.
Errea I, Rousseau B, and Bergara A.
Journal of Applied Physics 111, 112604 (2012).

Inertness and degradation of (0001) surface of Bi_2Se_3 topological insulator.
Golyashov VA, Kokh KA, Makarenko SV, Romanyuk KN, Prosvirin IP, Kalinkin AV, Tereshchenko OE, Kozhukhov AS, Sheglov DV, Eremeev SV, Borisova SD, and Chulkov EV.
Journal of Applied Physics 112, 113702 (2012).

The extended Koopmans' theorem: Vertical ionization potentials from natural orbital functional theory.
Piris M, Matxain JM, Lopez X, and Ugalde JM.
Journal of Chemical Physics 136, 174116 (2012).

Vibrational deexcitation and rotational excitation of H_2 and D_2 scattered from Cu(111): Adiabatic versus non-adiabatic dynamics.
Muzas AS, Juaristi JI, Alducin M, Díez Muiño R, Kroes GJ, and Díaz C.
Journal of Chemical Physics 137, 064707 (2012).

Dynamical reaction pathways in Eley-Rideal recombination of nitrogen from W(100).
Quintas-Sanchez E, Larregaray P, Crespos C, Martin-Gondre L, Rubayo-Soneira J, and Rayez JC.
Journal of Chemical Physics 137, 064709 (2012).

Component dynamics in polyvinylpyrrolidone concentrated aqueous solutions.
Busselez R, Arbe A, Cerveny S, Capponi S, Colmenero J, and Frick B.
Journal of Chemical Physics 137, 084902 (2012).

Cluster glasses of ultrasoft particles.
Coslovich D, Bernabei M, and Moreno AJ.
Journal of Chemical Physics 137, 184904 (2012).

Non-adiabatic effects within a single thermally averaged potential energy surface: Thermal expansion and reaction rates of small molecules.
Alonso JL, Castro A, Clemente-Gallardo J, Echenique P, Mazo JJ, Polo V, Rubio A, and Zueco D.
Journal of Chemical Physics 137, 184904 (2012).

Performance of PNOF5 natural orbital functional for radical formation reactions: hydrogen atom abstraction and C-C and O-O homolytic bond cleavage in selected molecules.
Lopez X, Ruiperez F, Piris M, Matxain JM, Matito E, and Ugalde, JM.
Journal of Chemical Theory and Computation 8, 2646 (2012).

Molecular diversity, metabolic transformation, and evolution of carotenoid feather pigments in cotingas (Aves: Cotingidae).
Prum RO, LaFountain, AM Berro J, Stoddard MC, and Frank HA.
Journal of Comparative Physiology B-Biochemical Systemic and Environmental Physiology 182, 1095 (2012).

Electron-pair density decomposition for core-valence separable systems.
Wang J, Wang Y, and Ugalde JM.
Journal of Computational Chemistry 33, 2243 (2012).

Lifetimes of electronic excitations in unoccupied surface states and the image potential states on Pd(110).
Tsirkin SS, Eremeev SV, and Chulkov, EV.
Journal of Experimental and Tehoretical Physics 115, 673 (2012).

Pro-oxidant activity of aluminum: Promoting the Fenton reaction by reducing Fe(III) to Fe(II).
Ruiperez F, Mujika JI, Ugalde JM, Exley C, and Lopez X.
Journal of Inorganic Biochemistry 117, 118 (2012).

Spectroscopy of thulium and holmium heavily doped tellurite glasses.
Gebavi H, Milanese D, Balda R, Taccheo S, Fernandez J, Lousteau J, and Ferraris M.
Journal of Luminescence 132, 270 (2012).

Hybrid organic/inorganic semiconductor nanostructures with highly efficient energy transfer.
Savateeva D, Melnikau D, Lesnyak V, Gaponik N and Rakovich YP.
Journal of Materials Chemistry 22, 10816 (2012).

Semiconductor nanowires self-assembled from colloidal CdTe nanocrystal building blocks: optical properties and application perspectives.
Rakovich YP, Jackel F, Donegan JF, and Rogach AL.
Journal of Materials Chemistry 22, 20831 (2012).

A first-principles study of II-VI (II = Zn; VI = O, S, Se, Te) semiconductor nanostructures.
Azpiroz JM, Infante I, Lopez X, Ugalde JM, and De Angelis F.
Journal of Materials Chemistry 22, 21453 (2012).

Moments of powers of the Hulthen density.
Glasser ML, and Nagy I.
Journal of Mathematical Chemistry 50, 1707 (2012).

Evolutionary continuous cellular automaton for the simulation of wet etching of quartz.
Ferrando N, Gosalvez MA, and Colom RJ.
Journal of Micromechanics and Microengineering 22, 025021 (2012).

Etched profile control in anisotropic etching of silicon by TMAH plus Triton.
Pal P, Gosalvez MA, and Sato K.
Journal of Micromechanics and Microengineering 22, 065013 (2012).

Evolutionary determination of kinetic Monte Carlo rates for the simulation of evolving surfaces in anisotropic etching of silicon.
Xing Y, Gosalvez MA, Sato K, Tian M, and Yi H.
Journal of Micromechanics and Microengineering 22, 085020 (2012).

Solvent effect on cation-pi interactions with Al^{3+}.
Larrucea, J.
Journal of Molecular Modeling 18, 4349 (2012).

The effect of ZnF_2 on the near-infrared luminescence from thulium doped tellurite glasses.
Gebavi H, Taccheo S, Balda R, Fernandez JM, Milanese D, Auzel F.
Journal of Non-crystalline Solids 358, 1497 (2012).

QTAIM characteristics of halogen bond and related interactions.
Grabowski SJ.
Journal of Physical Chemistry A 116, 1838 (2012).

Strain-Tunable spin moment in Ni-doped graphene.
Santos EJG, Ayuela A, and Sanchez-Portal D.
Journal of Physical Chemistry C 116, 1174 (2012).

Quasiclassical trajectory dynamics study of atomic oxygen collisions on an O-preadsorbed graphite (0001) surface with a new analytical potential energy surface.
Morón V, Martin-Gondre L, Crespos C, Gamallo P, and Sayós R.
Journal of Physical Chemistry C 116, 13092 (2012).

Electronic structure of diamond surfaces functionalized by $Ru(tpy)_2$.
Zegkinoglou I, Cook PL, Johnson PS, Yang WL, Guo JH, Pickup D, Gonzalez-Moreno R, Rogero C,Ruther RE, Rigsby ML, Ortega JE, Hamers RJ, and Himpsel FJ.
Journal of Physical Chemistry C 116, 13877 (2012).

Glycine adsorption at nonstoichiometric (010) hydroxyapatite surfaces: A B3LYP study.
Jimenez-Izal E, Chiatti F, Corno M, Rimola A, and Ugliengo P.
Journal of Physical Chemistry C 116, 14561 (2012).

Coordinated H-Bonding between porphyrins on metal surfaces.
Garcia-Lekue A, Gonzalez-Moreno R, Garcia-Gil S, Pickup DF, Floreano L, Verdini A, Cossaro A, Martin-Gago JA, Arnau A and Rogero C.
Journal of Physical Chemistry C 116, 15378 (2012).

Understanding charge transfer in donor–acceptor/metal systems: a combined theoretical and experimental study.
Cabellos JL, Mowbray DJ, Goiri E, El-Sayed, Floreano L, de Oteyza DG, Rogero C, Ortega JE, and Rubio A.
Journal of Physical Chemistry C 116, 17991 (2012).

The nature of radiative transitions in TiO_2-based nanosheets.
Palummo M, Giorgi G, Chiodo L, Rubio A, and Yamashita K.
Journal of Physical Chemistry C 116, 18495 (2012).

Dynamics of the oxygen molecules scattered from the graphite (0001) surface and comparison with experimental data.
Morón V, Martin-Gondre L, Gamallo P, and Sayós R.
Journal of Physical Chemistry C 116, 21482 (2012).

Dynamics of Nitrogen Scattering off N-Covered Ag(111).
Blanco-Rey M, Martin-Gondre L, Díez Muiño R, Alducin M, and Juaristi JI.
Journal of Physical Chemistry C 116, 21903 (2012).

Dielectric study of hydration water in silica nanoparticles.
Cerveny S, Schwartz GA, Otegui J, Colmenero J, Loichen J, and Westermann S.
Journal of Physical Chemistry C 116, 24340 (2012).

Bonding and charge transfer in metal-organic coordination networks on Au(111) with strong acceptor molecules.
Faraggi MN, Jiang N, Gonzalez-Lakunza N, Langner A, Stepanow S, Kern K, and Arnau A.
Journal of Physical Chemistry C 116, 24558 (2012).

Simple composite dipole model for the 0ptical modes of strongly-coupled plasmonic nanoparticle aggregates.
Taylor RW, Esteban R, Mahajan S, Coulston R, Scherman OA, Aizpurua J, and Baumberg JJ.
Journal of Physical Chemistry C 116, 25044 (2012).

Modeling surface passivation of ZnS quantum dots.
Azpiroz JM, Lopez X, Ugalde JM, and Infante I.
Journal of Physical Chemistry C 116, 2740 (2012).

Supramolecular environment-dependent electronic properties of metal-organic interfaces.
El-Sayed A, Mowbray DJ, Garcia-Lastra JM, Rogero C, Goiri E, Borghetti P, Turak A, Doyle BP, Dell'Angela M, Floreano L, Wakayama Y, Rubio A, Ortega JE, and de Oteyza DG.
Journal of Physical Chemistry C 116, 4780 (2012).

Magnetism of single vacancies in rippled graphene.
Santos EJG, Riiikonen S, Sanchez-Portal D, and Ayuela A.
Journal of Physical Chemistry C 116, 7602 (2012).

Structural and optoelectronic properties of unsaturated ZnO and ZnS nanoclusters.
Malloci G, Chiodo L, Rubio A, and Mattoni, A.
Journal of Physical Chemistry C 116, 8741 (2012).

^{29}Si NMR in cement: A theoretical study on calcium silicate hydrates.
Rejmak P, Dolado JS, Stott MJ, and Ayuela A.
Journal of Physical Chemistry C 116, 9755 (2012).

Multiscale theoretical modeling of plasmonic sensing of hydrogen uptake in palladium nanodisks.
Ameen Poyli M, Silkin VM, Chernov IP, Echenique PM, Díez Muiño R, and Aizpurua J.
Journal of Physical Chemistry Letters 3, 2556 (2012).

Understanding periodic dislocations in 2D supramolecular crystals: The PFP/Ag(111) interface.
Goiri E, Garcia-Lastra JM, Corso M, El-Fattah ZMA, Ortega JE, and de Oteyza DG.
Journal of Physical Chemistry Letters 3, 848 (2012).

The helium atom in metallic electron gases: a comparative study based on screened Schrödinger Hamiltonians.
Nagy I, Aldazabal I and Glasser ML.
Journal of Physics B: Atomic, Molecular and Optical Physics 45, 095701 (2012).

Ettringite strengthening at high pressures induced by the densification of the hydrogen bond network.
Manzano H, Ayuela A, Telesca A, Monteiro PJM, and Dolado JS.
Journal of Physics Chemistry C 116, 16138 (2012).

Time-dependent density-functional theory in massively parallel computer architectures: the OCTOPUS project.
Andrade X, Alberdi-Rodriguez J, Strubbe DA, Oliveira MJT, Nogueira F, Castro A, Muguerza J, Arruabarrena A, Louie SG, Aspuru-Guzik A, Rubio A, and Marques, MAL.
Journal of Physics Condensed Matter 24, 233202 (2012).

Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters.
Perdew JP, Tao JM, Hao P, Ruzsinszky A, Csonka GI, and Pitarke JM.
Journal of Physics Condensed Matter 24, 424207 (2012).

Anomalous photon-assisted tunneling in graphene.
Iurov A, Gumbs G, Roslyak O, and Huang DH.
Journal of Physics-Condensed Matter 24, 015303 (2012).

Comparative study of vibrations in submonolayer structures of potassium on Pt(111).
Rusina, GG, Eremeev SV, Borisova SD, and Chulkov EV.
Journal of Physics-Condensed Matter 24, 104003 (2012).

Positron annihilation and relaxation dynamics from dielectric spectroscopy: poly(vinylmethylether).
Bartos J, Iskrova-Miklosovicova M, Cangialosi D, Alegria A, Sausa O, Svajdlenkova H, Arbe A, Kristiak J, and Colmenero J.
Journal of Physics-Condensed Matter 24, 155104 (2012).

Surface phonons on Pb(111).
Sklyadneva IY, Heid R, Bohnen K-P, Echenique PM, and Chulkov EV.
Journal of Physics: Condensed Matter 24, 104004 (2012).

Tuning the plasmon energy of palladium-hydrogen systems by varying the hydrogen concentration.
Silkin VM, Díez Muiño R, Chernov IP, Chulkov EV, and Echenique PM.
Journal of Physics: Condensed Matter 24, 104021 (2012).

Effect of surface reconstruction on the photoemission cross-section of the Au(111) surface state.
Borghetti P, Lobo-Checa J, Goiri E, Mugarza A, Schiller F, Ortega JE, and Krasovskii EE.
Journal of physics. Condensed Matter: an Institute of Physics Journal 24, 395006 (2012).

Plasmon tsunamis on metallic nanoclusters.
Lucas AA and Sunjic M.
Journal of Physics. Condensed Matter: an Institute of Physics journal 24, 104022 (2012).

Karl-Heinz Rieder: the quiet pioneer.
Benedek G.
Journal of Physics. Condensed Matter: an Institute of Physics Journal 24, 350401 (2012).

Electron-phonon relaxation and excited electron distribution in zinc oxide and anatase.
Zhukov VP, Tyuterev VG, and Chulkov EV.
Journal of Physics. Condensed matter: an Institute of Physics Journal 24, 405802 (2012).

The storage of hydrogen in nanoporous carbons.
Alonso JA, Cabria,I, and López MJ.
Journal of the Mexican Chemical Society 56(3), 261 (2012).

Structure and optical function of amorphous photonic nanostructures from avian feather barbs: a comparative small angle X-ray scattering (SAXS) analysis of 230 bird species.
Saranathan V, Forster JD, Noh H, Liew SF, Mochrie SGJ, Hui Cao, Dufresne ER, and Prum RO.
Journal of the Royal Society Interface 9, 2563 (2012).

Variation in carotenoid-protein interaction in bird feathers produces novel plumage coloration.
Mendes-Pinto MM, LaFountain AM, Stoddard MC, Prum RO, Frank HA, and Robert, B.
Journal of the Royal Society Interface 9, 3338 (2012).

How chain plasmons govern the optical response in strongly interacting self-assembled metallic clusters of nanoparticles.
Esteban R, Taylor RW, Baumberg JJ, and Aizpurua J.
Langmuir, 28, 8881 (2012).

Neutron scattering and X-ray investigation of the structure and dynamics of poly (ethyl methacrylate).
Genix AC, Arbe A, Colmenero J, Wuttke J, and Richter D.
Macromolecules 45, 2522 (2012).

Two-dimensional subnanometer confinement of Ethylene Glycol and Poly(ethylene oxide) by neutron spectroscopy: molecular size effects.
Barroso-Bujans F, Fernandez-Alonso F, Cerveny S, Arrese-Igor S, Alegria A, and Colmenero J.
Macromolecules 45, 3137 (2012).

Quasielastic Neutron Scattering Study on the Dynamics of Poly(alkylene oxide)s.
Gerstl C, Schneider GJ, Fuxman A, Zamponi M, Frick B, Seydel T, Koza M, Genix AC, Allgaier J, Richter D, Colmenero J, and Arbe A.
Macromolecules 45, 4394 (2012).

Unexpected PDMS behavior in segregated cylindrical and spherical nanophases of PS-PDMS asymmetric diblock copolymers.
del Valle-Carrandi L, Alegria A, Arbe A, and Colmenero J.
Macromolecules 45, 491 (2012).

Enthalpy recovery in nanometer to micrometer thick polystyrene films.
Boucher VM, Cangialosi D, Alegria A, and Colmenero J.
Macromolecules 45, 5296 (2012).

Single chain dynamic structure factor of poly(ethylene oxide) in dynamically asymmetric blends with poly(methyl methacrylate). Neutron scattering and molecular dynamics simulations.
Brodeck M, Alvarez F, Colmenero J, and Richter D.
Macromolecules 45, 536 (2012).

Short and intermediate range order in poly(alkylene oxide)s.
A neutron diffraction and molecular dynamics simulation study.
Gerstl C, Brodeck M, Schneider GJ, Su Y, Allgaier J, Arbe A, Colmenero J, and Richter D.
Macromolecules 45, 7293 (2012).

Heterogeneity of the segmental dynamics in cylindrical and spherical phases of diblock copolymers.
Slimani MZ, Moreno AJ, and Colmenero J.
Macromolecules 45, 8841 (2012).

Plasmonic excitation and manipulation with an electron beam.
Ernst J, Vesseur R, Aizpurua J, Coenen T, Reyes-Coronado A, Batson PE, and Polman A.
MRS Bulletin 37, 752 (2012).

Quantum plasmonics: nonlinear effects in the field enhancement of a plasmonic nanoparticle dimer.
Marinica DC, Kazansky AK, Nordlander P, Aizpurua J, and Borisov AG.
Nano Letters 12, 1333 (2012).

Intrinsic terahertz plasmons and magnetoplasmons in large scale monolayer graphene.
Crassee I, Orlita M, Potemski M, Walter AL, Ostler M, Seyller T, Gaponenko I, Chen J, and Kuzmenko, AB.
Nano Letters 12, 2470 (2012).

Artificially stacked atomic layers: toward new van der Waals solids.
Gao GH, Gao W, Cannuccia E, Taha-Tijerina J, Balicas L, Mathkar A, Narayanan TN, Liu Z, Gupta BK, Peng J, Yin YS, Rubio A, and Ajayan PM.
Nano Letters 12, 3518 (2012).

Dynamic screening of a localized hole during photoemission from a metal cluster.
Koval NE, Sanchez-Portal D, Borisov AG, and Díez Muiño R .
Nanoscale Research Letters 7, 447 (2012).

Optical nano-imaging of gate-tunable graphene plasmons.
Chen JN, Badioli M, Alonso-Gonzalez P, Thongrattanasiri S, Huth F, Osmond J, Spasenovic M, Centeno A, Pesquera A, Godignon P, Elorza AZ, Camara N, de Abajo FJG, Hillenbrand R, and Koppens FHL.
Nature 487, 77 (2012).

Revealing the quantum regime in tunnelling plasmonics.
Savage KJ, Hawkeye MM, Esteban E, Borisov AG, Aizpurua J, and Baumberg JJ.
Nature 491, 574 (2012).

Atom-specific spin mapping and buried topological states in a homologous series of topological insulators.
Eremeev SV, Landolt G, Menshchikova TV, Slomski B, Koroteev YM, Aliev ZS, Babanly MB, Henk J, Ernst A, Patthey L, Eich A, Ako Khajetoorians A, Hagemeister J, Pietzsch O, Wiebe J, Wiesendanger R, Echenique PM, Tsirkin SS, Amiraslanov IR, Dil JH, and Chulkov EV.
Nature Communications 3, 635 (2012).

Magnetic and electric coherence in forward- and back-scattered electromagnetic waves by a single dielectric subwavelength sphere.
Geffrin JM, Garcia-Camara B, Gomez-Medina R, Albella P, Froufe-Perez LS, Eyraud C, Litman A, Vaillon R, Gonzalez F, Nieto-Vesperinas M, Saenz JJ, and Moreno F.
Nature Communications 3, 1171 (2012).

Resolving the electromagnetic mechanism of surface-enhanced light scattering at single hot spots.
Alonso-Gonzalez P, Albella P, Schnell M, Chen J, Huth F, Garcia-Etxarri A, Casanova F, Golmar F, Arzubiaga L, Hueso LE, Aizpurua J, and Hillenbrand R.
Nature Communications 3, 684 (2012).

Bridging quantum and classical plasmonics with a quantum-corrected model.
Esteban R, Borisov AG, Nordlander P, and Aizpurua J.
Nature Communications 3, 825 (2012).

H-atom relay reactions in real space.
Kumagai T, Shiotari A, Okuyama H, Hatta S, Aruga T, Hamada I, Frederiksen T and Ueba H.
Nature Materials 11, 167 (2012).

Dielectric nanoparticles polarizability reveals identity.
Sahagún E, and Sáenz JJ.
Nature Materials 11, 748 (2012).

Ultrafast X-ray pulse characterization at free-electron lasers.
Grguras I, Maier AR, Behrens C, Mazza T, Kelly TJ, Radcliffe P, Dusterer S, Kazansky AK, Kabachnik NM, Tschentscher T, Costello JT, Meyer M, Hoffmann MC, Schlarb H and Cavalieri AL.
Nature Photonics 6, 851 (2012).

The geyser effect in the vacuum expansion of solid $^{3}He_{0.54}$ $^{4}He_{0.46}$ and the determination of the poisson ratio.
Nieto P, Benedek G, and Toennies JP.
New Journal of Physics 14, 013007 (2012).

Non-adiabatic effects during the dissociative adsorption of O_2 at Ag(111)? A first-principles divide and conquer study.
Goikoetxea I, Beltrán J, Meyer J, Juaristi JI, Alducin M, and Reuter K.
New Journal of Physics 14, 013050 (2012).

Sp magnetism in clusters of gold thiolates.
Ayuela A, Crespo P, García MA, Hernando A, and Echenique PM.
New Journal of Physics 14, 013064 (2012).

Attostreaking with metallic nano-objects.
Borisov AG, Echenique PM, and Kazansky AK.
New Journal of Physics 14, 023036 (2012).

Universal magnetic properties of sp^3-type defects in covalently functionalized graphene.
Santos EJG, Ayuela A, and Sanchez-Portal D.
New Journal of Physics 14, 043022 (2912).

Enhanced excitonic effects in the energy loss spectra of LiF and Ar at large momentum transfer.
Sharma S, Dewhurst JK, Sanna A, Rubio A, and Gross EKU.
New Journal of Physics 14, 053052 (2012).

Force and conductance during contact formation to a C60 molecule.
Hauptmann N, Mohn F, Gross L, Meyer G, Frederiksen T, and Berndt R.
New Journal of Physics 14, 073032 (2012).

Thermalization in systems with bipartite eigenmode entanglement.
Chung MC, Iucci A, and Cazalilla MA.
New Journal of Physics 14, 075013 (2012).

Ion energetics in electron-rich nanoplasmas.
Heidenreich A, Infante I, and Ugalde JM.
New Journal of Physics 14, 075017 (2012).

Unconventional spin texture of a topologically nontrivial semimetal Sb(110).
Strozecka A, Eiguren A, Bianchi M, Guan D, Voetmann CH, Bao S, Hofmann P, and Pascual, JI.
New Journal of Physics 14, 103026 (2012).

The effect of van der Waal's gap expansions on the surface electronic structure of layered topological insulators.
Eremeev SV, Vergniory MG, Menshchikova TV, Shaposhnikov AA, and Chulkov, EV.
New Journal of Physics 14, 113030 (2012).

Characterization of TiO_2 atomic crystals for nanocomposite materials oriented to optoelectronics.
Chiodo L, Massaro A, Laricchia S, Della Sala F, Cingolani R, Salazar M, Romero AH, and Rubio A.
Optical and Quantum Electronics 44, 291 (2012).

Anti-Stokes laser-induced cooling in rare-earth doped low phonon materials.
Fernandez J, Garcia-Adeva AJ, and Balda R.
Optical Materials 34, 579 (2012).

Site-selective laser spectroscopy of Nd^{3+} ions in $0.8CaSiO_3$-$0.2Ca_3(PO_4)_2$ biocompatible eutectic glass-ceramics.
Sola D, Balda R, Pena JI, and Fernandez J.
Optics Express 20, 10701 (2012).

Dielectric antennas - a suitable platform for controlling magnetic dipolar emission.
Schmidt MK, Esteban R, Sáenz JJ, Suárez-Lacalle I, Mackowski S, and Aizpurua J.
Optics Express 20, 13636 (2012).

Laser action in Nd^{3+}-doped lanthanum oxysulfide powders.
Iparraguirre I, Azkargorta J, Merdrignac-Conanec O, Al-Saleh M, Chlique C, Zhang XH, Balda R, and Fernandez J.
Optics Express 20, 23690 (2012).

A combination of concave/convex surfaces for field-enhancement optimization: the indented nanocone.
García-Etxarri A, Apell P, Käll M, and Aizpurua J.
Optics Express 20, 25201 (2012).

Stopping light in two dimensional quasicrystalline waveguides.
Trabattoni A, Maini L, and Benedek G.
Optics Express 20, 28267 (2012).

Detection of deep-subwavelength dielectric layers at terahertz frequencies using semiconductor plasmonic resonators.
Berrier A, Albella P, Ameen Poyli A, Ulbricht R, Bonn M, Aizpurua J, and Gomez Rivas J.
Optics Express 20, 5052 (2012).

Control of single emitter radiation by polarization- and position-dependent activation of dark antenna modes.
Schmidt MK, Mackowski S, and Aizpurua J.
Optics Letters 37, 1017 (2012).

Diffractive chains of plasmonic nanolenses: combining near-field focusing and collective enhancement mechanisms.
Almpanis E, Papanikolaou N, Auguié B, Tserkezis C, and Stefanou N.
Optics Letters 37, 4624 (2012).

Mechanism of C-terminal intein cleavage in protein splicing from QM/MM molecular dynamics simulations.
Mujika JI, Lopez X, and Mulholland AJ.
Organic Biomolecular Chemistry 10, 1207 (2012).

Temperature dependence of the liquid structure factor of dense monatomic fluids in the long wavelength limit in relation to thermal expansivity.
March NH, and Alonso JA.
Philosophical Magazine Letters 92, 133 (2012).

Complex spin texture in the pure and Mn-doped topological insulator Bi_2Te_3.
Henk J, Ernst A, Eremeev SV, Chulkov EV, Maznichenko IV, and Mertig I.
Physical Review Letters 108, 206801 (2012).

Optical properties of calcium under pressure from first-principles calculations.
Errea I, Rousseau B, Eiguren A, and Bergara A.
Physial Review B 86, 085106 (2012).

Electronic transport through ferromagnetic and superconducting junctions with spin-filter tunneling barriers.
Bergeret FS, Verso A, and Volkov AF.
Physical Review B 86, 214516 (2012).

Ab initio approach to the rate of radiative electron trapping and electron-hole recombination in B-, C-, and N-doped anatase.
Zhukov VP, and Chulkov EV.
Physica Status Solidi B-basic Solid State Physics 249, 1063 (2012).

Excited states of the green fluorescent protein chromophore: Performance of ab initio and semi-empirical methods.
Wanko M, Garcia-Risueno P, and Rubio A.
Physica Status Solidi B-Basic Solid State Physics 249, 392 (2012).

Sodium molecule on the surface of liquid helium-4 droplets: optical transitions probe collective excitations.
Tehver I, Hizhnyakov V, and Benedek G.
Physica Status Solidi C, 1 (2012).

Substitution effects on the absorption spectra of nitrophenolate isomers.
Wanko M, Houmoller J, Stochkel K, Suhr Kirketerp M, Petersen MAP, Nielsen MB, Nielsen SB, and Rubio A.
Physical Chemistry Chemical Physics : PCCP 14, 12905 (2012).

Transport properties of armchair graphene nanoribbon junctions between graphene electrodes.
Motta C, Sanchez-Portal D, and Trioni MI.
Physical Chemistry Chemical Physics 14, 10683 (2012).

Dielectric spectroscopy in the GHz region on fully hydrated zwitterionic amino acids.
Rodriguez-Arteche I, Cerveny S, Alegria A, and Colmenero J.
Physical Chemistry Chemical Physics 14, 11352 (2012).

CBe_5E- (E = Al, Ga, In, Tl): planar pentacoordinate carbon in heptaatomic clusters.
Castro AC, Martinez-Guajardo G, Johnson T, Ugalde JM, Wu YB, Mercero JM, Heine T, Donald KJ, and Merino, G.
Physical Chemistry Chemical Physics 14, 14764 (2012).

Dynamical behavior of highly concentrated trehalose water solutions: a dielectric spectroscopy study.
Pagnotta SE, Alegria A, and Colmenero J.
Physical Chemistry Chemical Physics 14, 2991 (2012).

An interpretation of the absorption and emission spectra of the gold dimer using modern theoretical tools.
Geethalakshmi KR, Ruiperez F, Knecht S, Ugalde JM, Morse MD, and Infante I.
Physical Chemistry Chemical Physics 14, 8732 (2012).

Dissociative and non-dissociative adsorption dynamics of N_2 on Fe(110).
Goikoetxea I, Alducin M, Díez Muiño R, and Juaristi JI.
Physical Chemistry Chemical Physics, 7471 (2012).

Aluminum speciation in biological environments.
The deprotonation of free and aluminum bound citrate in aqueous solution.
Mujika JI, Ugalde JM, and Lopez X.
Physical Chemistry Chemical Physics: 14, 12465 (2012).

A computational study on the intriguing mechanisms of the gas-phase thermal activation of methane by bare $[Ni(H)(OH)]^+$.
Lakuntza O, Matxain JM, Ruiperez F, Besora M, Maseras F, Ugalde JM, Schlangen M, and Schwarz H.
Physical Chemistry Chemical Physics: PCCP 14, 9306 (2012).

Self-assembling endohedrally doped CdS nanoclusters: new porous solid phases of CdS.
Jimenez-Izal E, Matxain JM, Piris M, and Ugalde JM.
Physical chemistry chemical physics: PCCP 14, 9676 (2012).

Series expansions for an exact two-electron wave function in terms of Lowdin's renormalized natural orbitals.
Nagy I, and Aldazabal I.
Physical Review A 85, 034501 (2012).

Band-structure effects in photoelectron-emission spectra from metal surfaces.
Rubiano CAR, Gravielle MS, Mitnik DM, and Silkin VM.
Physical Review A 85, 043422 (2012).

Dichroism in short-pulse two-color XUV plus IR multiphoton ionization of atoms.
Kazansky AK, Grigorieva AV, and Kabachnik NM.
Physical Review A 85, 053409 (2012).

Exact time evolution of the pair distribution function for an entangled two-electron initial state.
Nagy I, Aldazabal I, and Rubio A.
Physical Review A 86, 022512 (2012).

Effect of partial temporal coherence of XUV pulses in IR-laser-assisted photoionization.
Kazansky AK, Sazhina IP, and Kabachnik NM.
Physical Review A 86, 033404 (2012).

Orientation-dependent retarding force of a three-dimensional degenerate electron gas for slow homonuclear trimer.
Osmani O, and Nagy I.
Physical Review A 86, 042901 (2012).

Tuning the Kosterlitz-Thouless transition to zero temperature in anisotropic boson systems.
You JS, Lee H, Fang S, Cazalilla MA, and Wang DW.
Physical Review A, 043612 (2012).

Wannier-based calculation of the orbital magnetization in crystals.
Lopez MG, Vanderbilt D, Thonhauser T, and Souza, I.
Physical Review B 85, 014435 (2012).

Domain-wall-induced magnetoresistance in pseudo-spin-valve/superconductor hybrid structure
Suszka AK, Bergeret FS, and Berger A.
Physical Review B 85, 024529 (2012).

Self-consistent approach for spectral properties of single alkali adatoms on Cu(111).
Achilli S, Trioni MI, and Chulkov EV.
Physical Review B 85, 045408 (2012).

Efficient computation of magnon dispersions within time-dependent density functional theory using maximally localized Wannier functions.
Rousseau B, Eiguren A, and Bergara A.
Physical Review B 85, 054305 (2012).

Channeling of charge carrier plasmons in carbon nanotubes.
ramberger C, Roth F, Schuster R, Kraus R, Knupfer M, Einarsson E, Maruyama S, Mowbray DJ, Rubio A, and Pichler T.
Physical Review B 85, 085424 (2012).

Role of nonlocal exchange in the electronic structure of correlated oxides.
Iori F, Gatti M, and Rubio A.
Physical Review B 85, 115129 (2012).

Mean free path of a suddenly created fast electron moving in a degenerate electron gas.
Nagy I and Echenique PM.
Physical Review B 85, 115131 (2012).

Transformation of the Ag(111) surface state due to molecule-surface interaction with ordered organic molecular monolayers.
Zaitsev NL, Nechaev IA, Echenique PM, and Chulkov EV.
Physical Review B 85, 115301 (2012).

Spin-polarized states of matter on the surface of a three-dimensional topological insulator with implanted magnetic atoms.
Caprara, S, Tugushev VV, Echenique PM, and Chulkov EV.
Physical Review B 85, 121304 (R) (2012).

Electron localization in epitaxial graphene on Ru(0001) determined by moire corrugation.
Stradi D, Barja S, Diaz C, Garnica M, Borca B, Hinarejos JJ, Sanchez-Portal D, Alcami M, Arnau A, de Parga ALV, Miranda R, and Martin F.
Physical Review B 85, 121404 (2012).

Momentum-space finite-size corrections for quantum Monte Carlo calculations.
Gaudoin R, Gurtubay IG, and Pitarke JM.
Physical Review B 85, 125125 (2012).

Theory of orthogonal interactions of CO molecules on a one-dimensional substrate.
Lin CW, Feng M, Zhao J, Cabrera-Sanfelix P, Arnau A, Sanchez-Portal D, and Petek H.
Physical Review B 85, 125426 (2012).

Electron-phonon interaction in bulk Pb: beyond the Fermi surface.
Sklyadneva IY, Heid R, Echenique PM, Bohnen KB, and Chulkov EV.
Physical Review B 85, 155115 (2012).

Surface states on a topologically nontrivial semimetal: The case of Sb(110).
Bianchi M, Guan DD, Strozecka A, Voetmann CH, Bao SN, Pascual JI, Eiguren A, and Hofmann P.
Physical Review B 85, 155431 (2012).

Electron cooling in diffusive normal metal-superconductor tunnel junctions with a spin-valve ferromagnetic interlayer.
Ozaeta A, Vasenk, AS, Hekking FWJ and Bergeret FS.
Physical Review B 85, 174518 (2012).

Circuit quantum electrodynamics with a superconducting quantum point contact.
Romero G, Lizuain I, Shumeiko VS, Solano E, and Bergeret FS.
Physical Review B 85, 180506 (2012).

Laser-induced preferential dehydrogenation of graphane.
Zhang H, Miyamoto Y, and Rubio A.
Physical Review B 85, 201409 (2012).

Low-energy plasmonic structure in CaC_6.
Echeverry JP, Chulkov EV, Echenique PM, and Silkin, VM.
Physical Review B 85, 205135 (2012).

Quasiparticle interference on the surface of Bi_2Se_3 induced by cobalt adatom in the absence of ferromagnetic ordering.
Ye M, Eremeev SV, Kuroda K, Krasovskii EE, Chulkov EV, Takeda Y, Saitoh Y, Okamoto K, Zhu SY, Miyamoto K, Arita M, Nakatake M, Okuda T, Ueda Y, Shimada K, Namatame H, Taniguchi M, and Kimura A.
Physical Review B 85, 205317 (2012).

Momentum-resolved electron dynamics of image-potential states on Cu and Ag surfaces.
Schubert K, Damm A, Eremeev SV, Marks M, Shibuta M, Berthold W, Gudde J, Borisov AG, Tsirkin SS, Chulkov EV, and Hofer U.
Physical Review B 85, 205431 (2012).

Challenges in truncating the hierarchy of time-dependent reduced density matrices equations.
Akbari A, Hashemi MJ, Rubio A, Nieminen RM, and van Leeuwen R.
Physical Review B 85, 235121 (2012).

Van der Waals interaction in magnetic bilayer graphene nanoribbons.
Santos H, Ayuela A, Chico L, and Artacho E.
Physical Review B 85, 245430 (2012).

Role of band structure and local-field effects in the low-energy collective electronic excitation spectra of 2H-$NbSe_2$.
Faraggi MN, Arnau A, and Silkin VM.
Physical Review B 86, 035115 (2012).

Topology of spin polarization of the 5d states on W(110) and Al/W(110) surfaces.
Rybkin AG, Krasovskii EE, Marchenko D, Chulkov EV, Varykhalov A, Rader O, and Shikin AM.
Physical Review B 86, 035117 (2012).

Magnetic phases in the one-dimensional Kondo chain on a metallic surface.
Lobos AM, Cazalilla MA, and Chudzinski P.
Physical Review B 86, 035455 (2012).

Enhanced thermoelectric properties in hybrid graphene/boron nitride nanoribbons.
Yang KK, Chen YP, D'Agosta R, Xie YE, Zhong JX, and Rubio, A.
Physical Review B 86, 045425 (2012).

Spin-polarized Josephson and quasiparticle currents in superconducting spin-filter tunnel junctions.
Bergeret FS, Verso A, and Volkov AF.
Physical Review B 86, 060506 (2012).

Andreev current enhancement and subgap conductance of superconducting SFN hybrid structures in the presence of a small spin-splitting magnetic field.
Ozaeta A, Vasenko AS, Hekking FWJ, and Bergeret FS.
Physical Review B 86, 060509 (2012).

Plasmon dispersion in layered transition-metal dichalcogenides.
Cudazzo P, Gatti M, and Rubio A.
Physical Review B 86, 075121 (2012).

Anomalous insulator-metal transition in boron nitride-graphene hybrid atomic layers.
Song L, Balicas L, Mowbray DJ, Capaz RB, Storr K, Ci L, Jariwala D, Kurth S, Louie SG, Rubio A, and Ajayan PM.
Physical Review B 86, 075429 (2012).

Quantum-well states with image state character for Pb overlayers on Cu(111).
Zugarramurdi A, Zabala N, Silkin VM, Chulkov EV, and Borisov AG.
Physical Review B 86, 075434 (2012).

Phonons and electron-phonon interaction at the Sb(111) surface.
Campi D, Bernasconi M, and Benedek G.
Physical Review B 86, 075446 (2012).

Inversed linear dichroism in F K-edge NEXAFS spectra of fluorinated planar aromatic molecules.
de Oteyza DG, Sakko A, El-Sayed A, Goiri E, Floreano L, Cossaro A, Garcia-Lastra JM, Rubio A, and Ortega JE.
Physical Review B 86, 075469 (2012).

Unified description of ground and excited states of finite systems: The self-consistent GW approach.
Caruso F, Rinke P, Ren X, Scheffler M, and Rubio, A.
Physical Review B 86, 081102 (2012).

Temperature dependence of the dynamics of the first image-potential state on Ag(111).
Tsirkin SS, Eremeev SV, Chulkov EV, Marks M, Schubert K, Gudde J, and Höfer U.
Physical Review B 86, 085424 (2012).

Oxygen vibrations and acoustic surface plasmon on Be(0001).
Jahn M, Muller M, Endlich M, Néel N, Kröger J, Chis V, and Hellsing B.
Physical Review B 86, 085453 (2012).

Lattice dynamics of bismuth tellurohalides.
Sklyadneva IY, Heid R, Bohnen KP, Chis V, Volodin VA, Kokh KA, Tereshchenko OE, Echenique PM, and Chulkov EV.
Physical Review B 86, 094302 (2012).

Full magnetoelectric response of Cr_2O_3 from first principles.
Malashevich A, Coh S, Souza I, and Vanderbilt D.
Physical Review B 86, 094430 (2012).

LiB and its boron-deficient variants under pressure.
Hermann A, Suarez-Alcubilla A, Gurtubay IG, Yang LM, Bergara A, Ashcroft NW, and Hoffmann R.
Physical Review B 86, 144110 (2012).

Inelastic shot noise characteristics of nanoscale junctions from first principles.
Avriller R, and Frederiksen T.
Physical Review B 86, 155411 (2012).

Ab initio study of energy loss and wake potential in the vicinity of a graphene monolayer.
Despoja V, Dekanic K, Sunjic M, and Marusic L.
Physical Review B 86, 165419 (2012).

Vibrations in binary and ternary topological insulators: First-principles calculations and Raman spectroscopy measurements.
Chis V, Sklyadneva IY, Kokh KA, Volodin VA, Tereshchenko OE, and Chulkov EV.
Physical Review B 86, 174304 (2012).

Search for stable ferromagnets among A(IV)/Fe digital alloys (A(IV) = Si, Ge) using first-principles calculations.
Otrokov MM, Fischer G, Buczek P, Ernst A, and Chulkov EV.
Physical Review B 86, 184418 (2012).

Observation of a highly spin-polarized topological surface state in $GeBi_2Te_4$.
Okamoto K, Kuroda K, Miyahara H, Miyamoto K, Okuda T, Aliev ZS, Babanly MB, Amiraslanov IR, Shimada K, Namatame H, Taniguchi M, Samorokov DA, Menshchikova TV, Chulkov EV, and Kimura A.
Physical Review B 86, 195304 (2012).

Excitons in molecular crystals from first-principles many-body perturbation theory: picene versus pentacene.
Cudazzo P, Gatti M, and Rubio A.
Physical Review B 86, 195307 (2012).

Low-energy excitations in strongly correlated materials: A theoretical and experimental study of the dynamic structure factor in V_2O_3.
Iori F, Rodolakis F, Gatti M, Reining L, Upton M, Shvyd'ko Y, Rueff JP, and Marsi M.
Physical Review B 86, 205132 (2012).

Unoccupied topological states on bismuth chalcogenides.
Niesner D, Fauster T, Eremeev SV, Menshchikova TV, Koroteev YM, Protogenov AP, Chulkov EV, Tereshchenko OE, Kokh KA, Alekperov O, Nadjafov A, and Mamedov N.
Physical Review B 86, 205403 (2012).

Orbital polaron in double-exchange ferromagnets.
van den Berg TL, Lombardo P, Kuzian RO, and Hayn R.
Physical Review B 86, 235114 (2012).

Benchmark of GW methods for azabenzenes.
Marom N, Caruso F, Ren XG, Hofmann OT, Korzdorfer T, Chelikowsky JR, Rubio A, Scheffler M, and Rinke P.
Physical Review B 86, 245127 (2012).

Density functional theory analysis of flexural modes, elastic constants, and corrugations in strained graphene.
de Andres PL, Guinea F, and Katsnelson MI.
Physical Review B 86, 245409 (2012).

Nonequilibrium electron-vibration coupling and conductance fluctuations in a C60 junction.
Ulstrup S, Frederiksen T, and Brandbyge M.
Physical Review B 86, 245417 (2012).

Modifying the Cu(111) Shockley surface state by Au alloying.
Abd El-Fattah ZM, Matena M, Corso M, Ormaza M, Ortega JE, and Schiller F.
Physical Review B 86, 245418 (2012).

Electronic properties and lattice dynamics of the As(111) surface.
Campi D, Bernasconi M, and Benedek G.
Physical Review B 86, 245403 (2012).

TDDFT study of time-dependent and static screening in graphene.
Despoja V, Mowbray DJ, Vlahovic D and Marusic L.
Physical Review B 86, 195429 (2012).

Thermalization and quantum correlations in exactly solvable models.
Cazalilla MA, Iucci A, and Chung MC.
Physical Review E 85, 011133 (2012).

Time dependence of the segmental relaxation time of poly(vinyl acetate)-silica nanocomposites.
Boucher VM, Cangialosi D, Alegria A, and Colmenero J.
Physical Review E 86, 041501 (2012).

Time-resolved two-photon photoemission of unoccupied electronic states of periodically rippled graphene on Ru(0001).
Armbrust N, Gudde J, Jakob P, and Hofer U.
Physical Review Letters 108, 056801 (2012).

Angle-resolved electron spectroscopy of laser-assisted auger decay induced by a few-femtosecond X-ray pulse.
Meyer M, Radcliffe P, Tschentscher T, Costello JT, Cavalieri AL, Grguras I, Maier AR, Kienberger R, Bozek J, Bostedt C, Schorb S, Coffee R, Messerschmidt M, Roedig C, Sistrunk E, Di Mauro LF, Doumy G, Ueda K, Wada S Dusterer S, Kazansky AK,and Kabachnik NM.
Physical Review Letters 108, 063007 (2012).

Diffusion of hydrogen in Pd assisted by inelastic ballistic hot electrons.
Blanco-Rey M, Alducin M, Juaristi JI, and de Andres PL.
Physical Review Letters 108, 115902 (2012).

Detection of vibration-mode scattering in electronic shot noise.
Kumar M, Avriller R, Yeyati, AL, and van Ruitenbeek JM.
Physical Review Letters 108, 146602 (2012).

Proposal of a one-dimensional electron gas in the steps at the $LaAlO_3$-$SrTiO_3$ interface.
Bristowe NC, Fix T, Blamire MG, Littlewood PB, and Artacho E.
Physical Review Letters 108, 166802 (2012).

Experimental verification of $PbBi_2Te_4$ as a 3D topological insulator.
Kuroda K, Miyahara H, Ye M, Eremeev SV, Koroteev YM, Krasovskii EE, Chulkov EV, Hiramoto S, Moriyoshi C, Kuroiwa Y, Miyamoto K, Okuda T, Arita M, Shimada K, Namatame H, Taniguchi M, Ueda Y, and Kimura A.
Physical Review Letters 108, 206803 (2012).

Nonadiabatic Forces in Ion-Solid Interactions: The Initial Stages of Radiation Damage.
Correa AA, Kohanoff J, Artacho E, Sanchez-Portal D, and Caro A.
Physical Review Letters 108, 213201 (2012).

Electronic stopping power in gold: the role of d electrons and the H/He anomaly.
Zeb MA, Kohanoff J, Sanchez-Portal D, Arnau A, Juaristi JI, and Artacho E.
Physical Review Letters 108, 225504 (2012).

Ideal two-dimensional electron systems with a giant rashba-type spin splitting in real materials: surfaces of bismuth tellurohalides.
Eremeev SV, Nechaev IA, Koroteev YM, Echenique PM, and Chulkov EV.
Physical Review Letters 108, 246802 (2012).

Topological character and magnetism of the dirac state in Mn-Doped Bi_2Te_3.
Henk J, Flieger M, Maznichenko IV, Mertig I, Ernst A, Eremeev SV, and Chulkov EV.
Physical Review Letters 109, 076801 (2012).

Disentanglement of surface and bulk rashba spin splittings in noncentrosymmetric BiTeI.
Landolt G, Eremeev SV, Koroteev YM, Slomski B, Muff S, Neupert T, Kobayashi M, Strocov VN, Schmitt T, Aliev ZS, Babanly MB, Amiraslanov IR, Chulkov EV, Osterwalder J, and Dil JH.
Physical Review Letters 109, 116403 (2012).

$Ca_2Y_2Cu_5O_{10}$: The first frustrated quasi-1D ferromagnet close to criticality.
Kuzian RO, Nishimoto S, Drechsler S-L, Malek J, Johnston S, van den Brink J, Schmitt M, Rosner H, Matsuda M, Oka K, Yamaguchi H, and Ito T.
Physical Review Letters 109, 117207 (2012).

Density-functional theory for f-electron systems: the alpha-gamma phase transition in cerium.
Casadei M, Ren XG, Rinke P, Rubio A, and Scheffler M.
Physical Review Letters 109, 146402 82012).

Topological Surface States with Persistent High Spin Polarization across the Dirac Point in Bi_2Te_2Se and Bi_2Se_2Te.
Miyamoto K, Kimura A, Okuda T, Miyahara H, Kuroda K, Namatame H, Taniguchi M, Eremeev SV, Menshchikova TV, Chulkov EV, Kokh KA, and Tereshchenko OE.
Physical Review Letters 109, 166802 (2012).

Charge transport in azobenzene-based single-molecule junctions.
Kim Y, Garcia-Lekue A, Sysoiev D, Frederiksen T, Groth U, and Scheer E.
Physical Review Letters 109, 226801 (2012).

Van der Waals coefficients for nanostructures: fullerenes defy conventional wisdom.
Ruzsinszky A, Perdew JP, Tao JM, Csonka GI, and Pitarke JM.
Physical Review Letters 109, 233203 (2012).

Competition between electron and phonon excitations in the scattering of nitrogen atoms and molecules off tungsten and silver metal surfaces.
Martin-Gondre L, Alducin M, Bocan GA, Díez Muiño R and Juaristi JI.
Physical Review Letters 108, 096101 (2012).

Spin-Flip transitions induced by time-dependent electric fields in surfaces with strong spin-orbit interaction.
Ibañez-Azpiroz J, Eiguren A, Sherman EY, and Bergara A.
Physical Rewiev Letters 109, 156401 (2012).

Ab initio simulation of helium-ion microscopy images: the case of suspended graphene.
Zhang H, Miyamoto Y, and Rubio A.
Physical Review Letters 109, 265505 (2012).

Universal dynamical steps in the exact time-dependent exchange-correlation potential.
Elliott P,Fuks JI, Rubio A, and Maitra NT.
Physical Review Letters 109, 266404 (2012).

Enhanced physical aging of polymer nanocomposites: the key role of the area to volume ratio.
Cangialosi D, Boucher VM, Alegria A, and Colmenero J.
Polymer 53, 1362 (2012).

Maximally localized Wannier functions: Theory and applications.
Marzari N, Mostofi AA, Yates JR, Souza I, and Vanderbilt D.
Reviews of Modern Physics 84, 1419 (2012).

Sharp silicon tips with different aspect ratios in wet etching/DRIE and surfactant-modified TMAH etching.
Tang B, Sato K, and Gosalvez MA.
Sensors and Actuators A-Physical 188, 220 (2012).

Neutron scattering and molecular dynamics simulations: synergetic tools to unravel structure and dynamics in polymers.
Arbe A, Alvarez F, and Colmenero J.
Soft Matter 8 32, 8257 (2012).

Anomalous molecular weight dependence of chain dynamics in unentangled polymer blends with strong dynamic asymmetry.
Arrese-Igor S, Alegria A, Moreno AJ, and Colmenero J.
Soft Matter 8, 3739 (2012).

T-g depression and invariant segmental dynamics in polystyrene thin films.
Boucher VM, Cangialosi, D, Yin HJ, Schonhals A, Alegria, A, and Colmenero J.
Soft Matter 8, 5119 (2012).

Equilibrium exchange kinetics in n-alkyl-PEO polymeric micelles: single exponential relaxation and chain length dependence.
Zinn T, Willner L, Lund R, Pipich V, and Richter D.
Soft Matter 8, 623 (2012).

Pulse-induced nonequilibrium dynamics of acetylene inside carbon nanotube studied by an ab initio approach.
Miyamoto Y, Zhang H, and Rubio A.
The National Academy of Sciences of the United States of America 109, 8861 (2012).

Nanoparticle movement: Plasmonic forces and physical constraints.
Batson PE, Reyes-Coronado A, Barrera RG, Rivacoba A, Echenique PM, and Aizpurua J.
Ultramicroscopy 123, 50 (2012).

Michael nanocarriers mimicking transient-binding disordered proteins.
Sanchez-Sanchez A, Akbari S, Etxeberria A, Arbe A, Gasser U, Moreno AJ, Colmenero J, and Pomposo JA.
ACS Macro Letters 2, 491 (2013).

Endowing single-chain polymer nanoparticles with enzyme-mimetic activity.
Perez-Baena I, Barroso-Bujans F, Gasser U, Arbe A, Moreno AJ, Colmenero J, and Pomposo JA.
ACS Macro Letters 2, 775 (2013).

Large enhancement of nonlinear optical response in a hybrid nanobiomaterial consisting of bacteriorhodopsin and cadmium telluride quantum dots.
Rakovich A, Nabiev I, Sukhanova A, Lesnyak V, Gaponik N, Rakovich YP, and Donegan JF.
ACS Nano 7, 2154 (2013).

Tailored Formation of N-Doped Nanoarchitectures by Diffusion-Controlled on-Surface (Cyclo)-Dehydrogenation of Heteroaromatics.
Pinardi AL, Otero-Irurueta G, Palacio I, Martinez JI, Sanchez-Sanchez C, Tello M, Rogero C, Cossaro A, Preobrajenski A, Gomez-Lor B, Jancarik A, Stara IG, Stary I, Lopez MF, Mendez J, and Martin-Gago JA.
ACS Nano 7, 3676 (2013).

Octagonal defects as the source of gap states in graphene semiconducting structures.
El-Sayed A, Borghetti P, Goiri E, Rogero C, Floreano L, Lovat G, Mowbray DJ, Cabellos JL, Wakayama Y, Rubio A, Ortega JE, and de Oteyza DG.
ACS Nano 7, 6914 (2013).

Understanding energy-level alignment in donorcceptor/metal interfaces from core-level shifts.
Pelc M, Jaskolski W, Ayuela A, and Chico L.
Acta Physica Polonica A 124, 777 (2013).

Hydration and dynamic state of nanoconfined polymer layers govern toughness in nacre-mimetic nanocomposites.
Verho T, Karesoja M, Das P, Martikainen L, Lund R, Alegria A, Walther A, and Ikkala O.
Advanced Materials 25, 5055 (2013).

Phase-tunable colossal magnetothermal resistance in ferromagnetic Josephson valves.
Giazotto F, and Bergeret FS.
Applied Physics Letters 102, 132603 (2013).

Quantum interference hybrid spin-current injector.
Giazotto F, and Bergeret FS.
Applied Physics Letters 102, 162406 (2013).

Efficient electron refrigeration using superconductor/spin-filter devices.
Kawabata S, Ozaeta A, Vasenko AS, Hekking FWJ, and Bergeret, FS.
Applied Physics Letters 103, 032602 (2013).

Nanoscale texture development of C-S-H gel: A computational model for nucleation and growth.
Gonzalez-Teresa R, Dolado JS, Ayuela A, and Gimel JC.
Applied Physics Letters 103, 234105 (2013).

Thermal rectification of electrons in hybrid normal metal-superconductor nanojunctions.
Giazotto F, and Bergeret FS.
Applied Physics Letters 103, 242602 (2013).

SiGe quantum dots for fast hole spin Rabi oscillations.
Ares N, Katsaros G, Golovach VN, Zhang JJ, Prager A, Glazman LI, Schmidt OG, and De Franceschi S.
Applied Physics Letters 103, 263113 (2013).

Electronic structure of $SnSb_2Te_4$ and $PbSb_2Te_4$ topological insulators.
Menshchikova TV, Eremeev SV, and Chulkov EV.
Applied Surface Science 267, 1 (2013).

Bulk and surface electronic structure of $SnBi_4Te_7$ topological insulator.
Vergniory MG, Menshchikova TV, Eremeev SV, and Chulkov EV.
Applied Surface Science 267, 146 (2013).

Influence of the Ge-Sb sublattice atomic composition on the topological electronic properties of $Ge_2Sb_2Te_5$.
Silkin IV, Koroteev YM, Bihlmayer G, and Chulkov EV.
Applied Surface Science 267, 169 (2013).

Effective interactions of knotted ring polymers.
Narros A, Moreno AJ, and CN Likos.
Biochemical Society Transactions 41, 630 (2013).

Energy loss distribution of proton beams at normal incidence on multi-walled carbon nanotubes.
Valdés JE, Celedón C, Segura R, Abril I, Garcia-Molina R, Denton CD, Arista NR, and Vargas P.
Carbon 52, 137 (2013).

Combining stochastic and deterministic approaches within high efficiency molecular simulations.
Escribano B, Akhmatskaya E, and Mujika JI.
Central European Journal of Mathematics 11, 787 (2013).

Suitability of amorphous TiO_2 nanoparticles as a photoelectrode in dye sensitized solar cells: A DFT–TDDFT study.
Eithiraj RD, and Geethalakshmi KR.
Chemical Physics Letters 585, 138 (2013).

Aggregation and cooperative effects in the aldol reactions of lithium enolates.
Larranaga O, de Cozar A, Bickelhaupt FM, Zangi R, and Cossio, FP.
Chemistry - A European Journal 19, 13761 (2013).

Sigma-hole bond versus hydrogen bond: from tetravalent to pentavalent N, P, and As atoms.
Grabowski SJ.
Chemistry - A European Journal 19, 14600 (2013).

Computational study on the attack of COH radicals on aromatic amino acids.
Mujika JI, Uranga J, and Matxain JM.
Chemistry - A European Journal 19, 6862 (2013).

Structure, atomistic simulations, and phase transition of stoichiometric Yeelimite.
Cuesta A, De la Torre AG, Losilla ER, Peterson VK, Rejmak P, Ayuela A, Frontera C, and Aranda MAG.
Chemistry of Materials 25, 1680 (2013).

Quantum chemical study of the reactions between Pd^+/Pt^+ and H_2O/H_2S.
Lakuntza O, Matxain JM, Ruiperez F, Ugalde JM, and Armentrout PB.
Chemistry - A European Journal 19, 8832 (2013).

The isolation of single MMX chains from solution: unravelling the assembly-disassembly process.
Azani MR, Paz AP, Hermosa C, Givaja G, Gomez-Herrero J, Mas-Balleste R, Zamora F, and Rubio A.
Chemistry - A European Journal 19, 15518 (2013).

Simulating pump-probe photoelectron and absorption spectroscopy on the attosecond timescale with time-dependent density functional theory.
De Giovannini U, Brunetto G, Castro A, Walkenhorst J and Rubio A.
Chemphyschem 14, 1363 (2013).

Model for the formation of helium bubbles in palladium.
Alonso JA, and Ayuela A.
Croatica Chemica Acta 86, 4, 425 (2013).

Neel temperature of antiferromagnets for phase transitions driven by spin-wave interactions.
Ayuela A, Klein DJ, and March NH.
Croatica Chemica Acta 86, 4, 425 (2013).

Implementation and evaluation of the level set method: towards efficient and accurate simulation of wet etching for microengineering applications.
Montoliu C, Ferrando N, Gosálvez MA, Cerdáa J, and Colom RJ.
Computer Physics Communications 184, 2299 (2013).

Bounds on the PNOF5 natural geminal occupation numbers.
Piris M.
Computational and Theoretical Chemistry 1003, 123 (2013).

Low temperature red luminescence of a fluorinated Mn-doped zinc selenite.
Orive J, Balda R, Fernández J, Lezama L, and Arriortua MI.
Dalton Transactions 42, 12481 (2013).

One-step wet chemical deposition of NiO from the electrochemical reduction of nitrates in ionic liquid based electrolytes.
Azaceta E, Tuyen NT, Pickup DF, Rogero C, Ortega JE, Miguel O, Grande HJ, and Tena-Zaera R.
Electrochimica Acta 96, 261 (2013).

Energy-loss straggling of 2-10 MeV/u Kr ions in gases.
Vockenhuber C, Jensen J, Julin J, Kettunen H, Laitinen M, Rossi M, Sajavaara T, Osmani O, Schinner A, Sigmund P, and Whitlow HJ.
European Physical Journal D 67, 145 (2013).

Molecules with high Bond orders and ultrashort Bond lengths: CrU, MoU, and WU.
Ruiperez F, Merino G, Ugalde JM, and Infante I.
Inorganic Chemistry 52, 2838 (2013).

A natural orbital functional based on an explicit approach of the two electron cumulant.
Piris M.
International Journal of Quantum Chemistry 113, 620 (2013).

Efficient step-mediated intercalation of silver atoms deposited on the Bi_2Se_3 surface.
Otrokov MM, Borisova SD, Chis V, Vergniory MG, Eremeev SV, Kuznetsov VM, and Chulkov EV.
Jetp Letters 96, 714 (2013).

New topological surface state in layered topological insulators: Unoccupied dirac cone.
Eremeev SV, Silkin IV, Menshchikova TV, Protogenov AP, and Chulkov EV.
Jetp Letters 96, 780 (2013).

Many-body effects on the width of the band gap in Bi_2Te_2X (X = Te, Se, S) topological insulators.
Rusinov IP, Nechaev IA, and Chulkov EV.
Jetp Letters 98, 397 (2013).

Pressure induced phase transitions in TiH_2.
Gao GY, Bergara A, Liu GT, and Ma YM.
Journal of Applied Physics 113, 103512 (2013).

Structural and electronic properties of Ni_{26-pXp} clusters (X = Pd, Pt):
A density-functional-theory study.
Aguilera-Granja, and Gallego LJ.
Journal of Applied Physics 114, 054311 (2013).

Electronic structure of Fe- vs. Ru-based dye molecules.
Johnson PS, Cook PL, Zegkinoglou I, Garcia-Lastra JM, Rubio A, Ruther RE, Hamers RJ, and Himpsel FJ.
Journal of Chemical Physics 138, 044709 (2013).

On the interactions between poly(ethylene oxide) and graphite oxide:
comparative study by different computational methods.
Garcia-Yoldi I, Alvarez F, and Colmenero J.
Journal of Chemical Physics 138, 094308 (2013).

Communication: Chemical bonding in carbon dimer isovalent series from the
natural orbital functional theory perspective.
Matxain JM, Ruiperez F, Infante I, Lopez X, Ugalde JM, Merino G, and Piris M.
Journal of Chemical Physics 138, 151102 (2013).

Electronic spectroscopy and electronic structure of diatomic IrSi.
Garcia MA, Vietz C, Ruiperez F, Morse MD, and Infante I.
Journal of Chemical Physics 138, 154306 (2013).

Comment on "Unified explanation of the anomalous dynamic properties of
highly asymmetric polymer blends" [J. Chem. Phys. 138, 054903 (2013)].
Colmenero, J.
Journal of Chemical Physics 138, 197101 (2013).

Modeling the collective relaxation time of glass-forming polymers at intermediate length scales:
application to polyisobutylene.
Colmenero J, Alvarez F, Khairy Y, and Arbe A.
Journal of Chemical Physics 139, 044906 (2013).

Interpair electron correlation by second-order perturbative corrections to PNOF5.
Piris M.
Journal of Chemical Physics 139, 064111 (2013).

Determination of the surface structure of CeO_2(111) by low-energy electron diffraction.
Siegel DA, Chueh WC, El Gabaly F, McCarty KF, de la Figuera J, and Blanco-Rey M.
Journal of Chemical Physics 139, 114703 (2013).

Cause of the fragile-to-strong transition observed in water confined in C-S-H gel.
Monasterio M, Jansson H, Gaitero JJ, Dolado JS, and Cerveny S.
Journal of Chemical Physics 139, 164714 (2013).

Room temperature compressibility and diffusivity of liquid water from first principles.
Corsetti F, Artacho E, Soler JM, Alexandre SS, and Fernandez-Serra MV.
Journal of Chemical Physics 139, 194502 (2013).

The intrapair electron correlation in natural orbital functional theory.
Piris M, Matxain JM, and Lopez, X.
Journal of Chemical Physics 139, 234109 (2013).

Theoretical study of influencing factors on the dispersion of bulk band-gap edges and the surface
states in topological insulators Bi_2Te_3 and Bi_2Se_3.
Rusinov IP, Nechaev IA, and Chulkov EV.
Journal of Experimental and Theoretical Physics 116, 1006 (2013).

Design of solar cell materials via soft X-ray spectroscopy.
Himpsel FJ, Cook PL, de la Torre G, Garcia-Lastra JM, Gonzalez-Moreno R, Guo JH, Hamers RJ,
Kronawitter CX, Johnson PS, Ortega JE, Pickup D, Ragoussi ME, Rogero C, Rubio A, Ruther RE,
Vayssieres L, Yang W, and Zegkinoglou I.
Journal of Electron Spectroscopy and Spectroscopy and Related Phenomena 190, 2 (2013).

Formation of the OOH center dot radical at steps of the boehmite surface and its inhibition
by gallic acid: A theoretical study including DFT-based dynamics.
Ribeiro T, Motta A, Marcus P, Gaigeot MP, Lopez X, and Costa D.
Journal of Inorganic Biochemistry 128, 164 (2013).

Near-infrared emission and upconversion in Er^{3+}-doped TeO_2-ZnO-ZnF_2 glasses.
Miguel A, Morea R, Gonzalo J, Arriandiaga MA, Fernandez J, and Balda R.
Journal of Luminiscence 140, 38 (2013).

Atomic and electronic properties of quasi-one-dimensional MoS_2 nanowires.
Seivane LF, Barron H, Botti S, Marques MAL, Rubio A, and Lopez-Lozano X.
Journal of Materials Research 28, 240 (2013).

Explicit form of Pauli potential for direct derivation of pair density from a two-particle differential
equation for the quintet state of four electrons with harmonicinterparticle interactions.
Akbari A, Amovilli C, March NH, and Rubio A.
Journal of Mathematical Chemistry 51, 1462 (2013).

Theory and phenomenology for a variety of classical and quantum phase transitions.
March NH, and Zhang ZD.
Journal of Mathematical Chemistry 51, 1694 (2013).

A proposed family of variationally correlated first-order density matrices for spin-polarized
three-electron model atoms.
Akbari A, March NH and Rubio A.
Journal of Mathematical Chemistry 51, 763 (2013).

Level set implementation for the simulation of anisotropic etching: application to complex
MEMS micromachining.
Montoliu C, Ferrando N, Gosalvez MA, Cerda J, and Colom RJ.
Journal of Micromechanics and Microengineering 23, 075017 (2013).

Theoretical study of the pH-dependent antioxidant properties of vitamin C.
Mujika JI, and Matxain JM.
Journal of Molecular Modeling 19, 1945 (2013).

Heavy periodane.
Azpiroz JM, Moreno D, Ramirez-Manzanares A, Ugalde JM, Mendez-Rojas MA, and Merino G.
Journal of Molecular Modeling 19, 1953 (2013).

Computational study of Be_2 using Piris natural orbital functionals.
Matxain JM, Ruiperez F, and Piris M.
Journal of Molecular Modeling 19, 1967 (2013).

Non-covalent interactions - QTAIM and NBO analysis.
Grabowski SJ.
Journal of Molecular Modeling 19, 4713 (2013).

Influence of axial and peripheral ligands on the electronic structure of titanium phthalocyanines.
Pickup DF, Zegkinoglou I, Ballesteros B, Ganivet CR, Garcia-Lastra JM, Cook PL, Johnson PS,
Rogero C, de Groot F, Rubio A, de la Torre G, Ortega JE, and Himpsel FJ.
Journal of Physical Chemistry C 117, 4410 (2013).

Strong enhancement of circular dichroism in a hybrid material consisting of
J-aggregates and silver nanoparticles.
Melnikau D, Savateeva D, Gun'ko YK, and Rakovich YP.
Journal of Physical Chemistry C 117, 13708 (2013).

Complexes between dihydrogen and amine, phosphine, and arsine derivatives.
Hydrogen bond versus pnictogen interaction.
Grabowski SJ, Alkorta I, and Elguero J.
Journal of Physical Chemistry A 117, 3243 (2013).

Toward an Understanding of the Hydrogenation Reaction of MO_2 Gas-Phase Clusters
(M = Ti, Zr, and Hf).
Gonzalez-Navarrete P, Calatayud M, Andres J, Ruiperez F, and Roca-Sanjuan D.
Journal of Physical Chemistry A 117, 5354 (2013).

Spectroscopy of donor-pi-acceptor porphyrins for dye-sensitized solar cells.
Zegkinoglou I, Ragoussi ME, Pemmaraju CD, Johnson PS, Pickup DF, Ortega JE, Prendergast D,
de la Torre G, and Himpsel FJ.
Journal of Physical Chemistry C 117, 13357 (2013)

Interface dipole effects as a function of molecular tilt: mechanical of electron tunneling
through self-assembled monolayers?
Foti G, Sanchez-Portal D, Arnau A, and Frederiksen T.
Journal of Physical Chemistry C 117, 14272 (2013).

Role of the anchored groups in the bonding and self-organization of macrocycles:
carboxylic versus pyrrole groups.
Gonzalez-Moreno R, Garcia-Lekue A, Arnau A, Trelka M, Gallego JM, Otero R, Verdini A,
Sanchez-Sanchez C, de Andres PL, Martin-Gago JA, and Rogero C.
Journal of Physical Chemistry C 117, 7661 (2013).

^{29}Si chemical shift anisotropies in hydrated calcium silicates: a computational study.
Rejmak P, Dolado JS, Stott MJ, and Ayuela A.
Journal of Physical Chemistry C 117, 8374 (2013).

Performance of nonlocal optics when applied to plasmonic nanostructures.
Stella L, Zhang P, Garcia-Vidal FJ, Rubio A, and Garcia-Gonzalez P.
Journal of Physical Chemistry C 117, 8941 (2013).

Scattering of nitrogen atoms off Ag(111) surfaces: A theoretical study.
Martin-Gondre L, Bocan GA, Blanco-Rey M, Alducin M, Juaristi JI, and Muiño RD.
Journal of Physical Chemistry C 117, 9779 (2013).

Face-Selective etching of ZnO during attachment of dyes.
Palacios-Lidon E, Pickup DF, Johnson PS, Ruther RE, Tena-Zaera R, Hamers RJ, Colchero J, Himpsel FJ,
Ortega JE, and Rogero C.
Journal of Physical Chemistry C 117, 18414 (2013).

Preperation and investigation of quantum-dot-loaded hollow polymer microspheres.
Hanley CA, McCarthy JE, Purcell-Milton F, Gerard V, McCloskey D, Donegan J, Rakovich YP, and Gun'ko YK.
Journal of Physical Chemistry C 117, 24527 (2013).

Stark ionization of atoms and molecules within density functional resonance theory.
Larsen AH, De Giovannini U, Whitenack DL, Wasserman A, and Rubio A.
Journal of Physical Chemistry Letters 4, 2734 (2013).

Gold and methane: a noble combination for delicate oxidation.
Mowbray DJ, Migani A, Walther G, Cardamone DM, and Rubio A.
Journal of Physical Chemistry Letters 4, 3006 (2013).

Efficient N_2 formation on Ag(111) by Eley–Rideal recombination of hyperthermal atoms.
Blanco-Rey M, Díaz E, Bocan GA, Díez Muiño R, Alducin M, and Juaristi JI.
Journal of Physical Chemistry Letters 4, 3704 (2013).

Adiabatic energy loss in hyperthermal H atom collisions with Cu and Au:
a basis for testing the importance of nonadiabatic energy loss.
Pavanello M, Auerbach DJ, Wodtke AM, Blanco-Rey M, and Alducin M, and Kroges GJ.
Journal of Physical Chemistry Letters 4, 3735 (2013).

Dynamics of charge-transfer processes with time-dependent density functional theory.
Fuks JI, Elliott P, Rubio A, and Maitra NT.
Journal of Physical Chemistry Letters 4, 735 (2013).

Dihydrogen bond and X-H center dot center dot center dot sigma interaction as sub-classes of
hydrogen bond.
Grabowski SJ.
Journal of Physical Organic Chemistry 26, 452 (2013).

Influence of the partial temporal coherence of short FEL pulses on two-colour
photoionization and photoinduced Auger decay of atoms.
Kazansky AK, Sazhina IP, and Kabachnik NM.
Journal of Physics B-Atomic Molecular and Optical Physics 46, 025601 (2013).

Interference in the angular distribution of photoelectrons in superimposed XUV and optical laser fields.
Düsterer, Rading L, Johnsson P, Rouzée A, Hundertmark A, Vrakking MJJ, Radcliffe P, Meyer M,
Kazansky AK and Kabachnik NM.
Journal of Physics B-Atomic Molecular and Optical Physics 46, 164026 (2013).

Photoelectron angular distributions in infrared one-photon and two-photon ionization of
FEL-pumped Rydberg states of helium.
Mondal S, Fukuzawa H, Motomura K, Tachibana T, Nagaya K, Sakai T, Matsunami K, Yase S, Yao M,
Wada S, Hayashita H, Saito N, Callegari C, Prince KC, O'Keeffe P, Bolognesi P, Avaldi L, Miron C,
Nagasono M, Togashi T, Yabashi M, Ishikawa KL, Sazhina IP, Kazansky AK, Kabachnik NM, and Ueda K.
Journal of Physics B-Atomic Molecular and Optical Physics 46, 205601 (2013).

Low-loss electric and magnetic field-enhanced spectroscopy with subwavelength silicon dimers.
Albella P, Ameen Poyli M, Schmidt MK, Maier SA, Moreno F, Sáenz JJ, and Aizpurua J.
Journal of Physical Chemistry C 117, 13573 (2013).

Easy-axis ferromagnetic chain on a metallic surface.
Lobos AM, and Cazalilla MA.
Journal of Physics-Condensed Matter 25, 094008 (2013).

Hybridization between Cu-O chain and Cu(110) surface states in the O(2 x 1)/Cu(110) surface from first principles.
Cabrera-Sanfelix P, Lin CW, Arnau A, and Sanchez-Portal D.
Journal of Physics-Condensed Matter 25, 135003 (2013).

Anisotropy of spin relaxation and transverse transport in metals.
Mokrousov Y, Zhang HB, Freimuth F, Zimmermann B, Long NH, Weischenberg J, Souza I, Mavropoulos P, and Blugel S.
Journal of Physics-Condensed Matter 25, 163201 (2013).

Optimal finite-range atomic basis sets for liquid water and ice.
Corsetti F, Fernandez-Serra MV, Soler JM, and Artacho E.
Journal of Physics-Condensed Matter 25, 435504 (2013).

Photon dressed electronic states in topological insulators:tunneling and conductance.
Iurov A, Gumbs G, Roslyak and Huang D.
Journal of Physics: Condensed Matter 25, 135502 (2013)

Multiple excitation of Fuchs-Kliewer phonons by Ne(+) ions back-scattered by the LiF(100) surface at grazing incidence.
Lucas A A, Sunjic M, and Benedek G.
Journal of Physics. Condensed matter: an Institute of Physics Journal 25, 355009 (2013).

Volume recovery of polystyrene/silica nancomposites.
Cangialosi D, Boucher VM, Alegria A, and Colmenero J.
Journal of Polymer Science Part B-Polymer Physics 51, 847 (2013).

Recent progress on polymer dynamics by neutron scattering: From simple polymers to complex materials.
Colmenero J, and Arbe A.
Journal of Polymer Science Part B-Polymer Physics 51, 87 (2013).

Andreev current and subgap conductance of spin-valve SFF structures.
Vasenko AS, Ozaeta A, Kawabata S, Hekking FWJ, and Bergeret FS.
Journal of Superconfuctivity and Novel Magnetism 26, 1951 (2013).

Spectroscopy and energy transfer in Nd^{3+}/Yb^{3+} codoped chalcohalide glasses.
Miguel A, Fan B, Balda R, Zhang X, Fernández J, and Adam JL.
Journal of Non-Crystalline Solids 377, 110 (2013).

Level Alignment of a Prototypical Photocatalytic System: Methanol on TiO_2(110).
Migani A, Mowbray D, Iacomino A, Zhao J, Petek H, and Rubio A.
Journal of the American Chemical Society 135, 11429 (2013).

On the effect of a single solvent molecule on the charge-transfer band of a donor-acceptor anion.
Houmoller J, Wanko M, Stochkel K, Rubio A, and Nielsen SB.
Journal of the American Chemical Society 135, 6818 (2013).

Direct observation of the formation of surfactant micelles under nonisothermal conditions by synchrotron SAXS.
Jensen GV, Lund R, Gummel J, Monkenbusch M, Narayanan T, and Pedersen JS.
Journal of the American Chemical Society 135, 7214 (2013).

Reply to "Comment on 'A generalized rouse incoherent scattering function for chain dynamics of unentangled polymers in dynamically asymmetric blends.
Colmenero J.
Macromolecules 46, 8056 (2013).

Dynamics of poly(butylene oxide) well above the glass transition. A fully atomistic molecular dynamics simulation study.
Colmenero J, Brodeck M, Arbe A, and Richter D.
Macromolecules 46, 1678 (2013).

Thermal stability of polymers confined in graphite oxide.
Barroso-Bujans F, Alegria A, Pomposo JA, and Colmenero J.
Macromolecules 46, 1890 (2013).

Influence of water and filler content on the dielectric response of silica-filled rubber compounds.
Otegui J, Schwartz GA, Cerveny S, Colmenero J, Loichen J, and Westermann S.
Macromolecules 46, 2407 (2013).

Effects of knots on ring polymers in solvents of varying quality.
Narros A, Moreno AJ, and Likos CN.
Macromolecules 46, 3654 (2013).

Dynamics of branched polymers: a combined study by molecular dynamics simulations and tube theory.
Bacova P, Hawke LGD, Read DJ, and Moreno AJ.
Macromolecules 46, 4633 (2013).

Dynamic heterogeneity in random and gradient copolymers: a computational investigation.
Slimani MZ, Moreno AJ, Rossi G, and Colmenero J.
Macromolecules 46, 5066 (2013).

A generalized rouse incoherent scattering function for chain dynamics of unentangled polymers in dynamically asymmetric blends.
Colmenero J.
Macromolecules 46, 5363 (2013).

End-to-end vector dynamics of nonentangled polymers in lamellar block copolymer melts: the role of junction point motion.
Lund R, Barroso-Bujans F, Slimani MZ, Moreno AJ, Willner L, Richter D, Alegria A, and Colmenero J.
Macromolecules 46, 7477 (2013).

Study of the dynamic heterogeneity in poly(ethylene-ran-vinyl acetate) copolymer by using broadband dielectric spectroscopy and electrostatic force microscopy.
Kummali MM, Alegria A, Miccio LA, and Colmenero J.
Macromolecules 46, 7502 (2013).

Chain length effects on the dynamics of poly(ethylene oxide) confined in graphite oxide: a broadband dielectric spectroscopy study.
Barroso-Bujans F, Cerveny S, Alegria A,,and Colmenero J.
Macromolecules 46, 7932 (2013).

Architecture-induced size asymmetry and effective interactions of ring polymers: simulation and theory.
Narros A, Moreno AJ, and Likos CN.
Macromolecules 46, 9437 (2013).

Advantages of orthogonal folding of single polymer chains to soft nanoparticles.
Moreno AJ, Lo Verso F, Sanchez-Sanchez A, Arbe A, Colmenero J, and Pomposo JA.
Macromolecules 46, 9748 (2013).

Design and preparation of single-chain nanocarriers mimicking disordered proteins for combined delivery of dermal bioactive cargos.
Sanchez-Sanchez A, Akbari S, Moreno AJ, Lo Verso F, Arbe A, Colmenero J, and Pomposo JA.
Macromolecular Rapid Communications 34, 1681 (2013).

Conversion of laser energy to nuclear energy driven by Coulomb explosion of nanostructures.
Heidenreich A, Last I, Ron S, and Jortner J.
Molecular Physics 111, 2108 (2013).

Ultrafast nonlinear control of progressively loaded, single plasmonic nanoantennas fabricated using helium ion milling.
Wang Y, Abb M, Boden SA, Aizpurua J, de Groot CH, and Muskens OL.
Nano Letters 13, 5647 (2013).

Controlling subnanometer gaps in plasmonic dimers using graphene.
Mertens J, Eiden AL, Sigle DO, Huang F, Lombardo A, Sun Z, Sundaram RS, Colli A, Tserkezis C, Aizpurua J, Milana S, Ferrari AC, and Baumberg JJ.
Nano Letters 13, 5033 (2013).

Plexciton quenching by resonant electron transfer from quantum emitter to metallic nanoantenna.
Marinica DC, Lourenço-Martins H, Aizpurua J, and Borisov AG.
Nano Letters 13, 5972 (2013).

Band structure engineering in topological insulator based heterostructures.
Menshchikova TV, Otrokov MM, Tsirkin SS, Samorokov DA, Bebneva VV, Ernst A, Kuznetsov VM, and Chulkov EV.
Nano Letters 13, 6064 (2013).

Snapshots of Dirac Fermions near the Dirac point in topological insulators.
Luo CW, Wang HJ, Ku SA, Chen HJ, Yeh TT, Lin JY, Wu KH, Juang JY, Young BL, Kobayashi T, Cheng CM, Chen CH, Tsuei KD, Sankar R, Chou FC, Kokh KA, Tereshchenko OE, Chulkov EV, Andreev YM, and Gu GD.
Nano Letters 13, 5797 (2013).

Metallicity retained by covalent functionalization of graphene with phenyl groups.
Tang PZ, Chen PC, Wu J, Kang FY, Li J, Rubio A, and Duan WH.
Nanoscale 5, 7537 (2013).

Resonance energy transfer in self-organized organic/inorganic dendrite structures.
Melnikau D, Savateeva D, Lesnyak V, Gaponik N, Nuñez Fernandez Y, Vasilevskiy MI, Costa MF, Mochalov KE, Oleinikov V, and Rakovich YP.
Nanoscale 5, 9317 (2013).

Strong plasmon-exciton coupling in a hybrid system of gold nanostars and J-aggregates.
Melnikau D, Savateeva D, Susha A, Rogach AL, and Rakovich YP.
Nanoscale Research Letters 8, 134 (2013).

Chemical mapping of a single molecule by plasmon-enhanced Raman scattering.
Zhang R, Zhang Y, Dong ZC, Jiang S, Zhang C, Chen LG, Zhang L, Liao Y, Aizpurua J, Luo Y, Yang JL, and Hou JG.
Nature 498, 82 (2013).

Quantum coherence controls the charge separation in a prototypical artificial light-harvesting system.
Rozzi CA, Falke SM, Spallanzani N, Rubio A, Molinari E, Brida D, Maiuri M, Cerullo G, Schramm H, Christoffers J, and Lienau C.
Nature Communications 4, 1602 (2013).

Coexisting massive and massless Dirac fermions in symmetry-broken bilayer graphene.
Su Kim K, L. Walter A, Moreschini L, Seyller T, Horn K, Rotenberg E, and Bostwick A.
Nature Materials 12, 887 (2013).

Optically induced 'negative forces'.
Dogariu A, Sukhov S, and Sáenz JJ.
Nature Photonics 7, 24 (2013).

Small scale rotational disorder observed in epitaxial graphene on SiC(0001).
Walter AL, Bostwick A, Speck F, Ostler M, Kim KS, Chang YJ, Moreschini L, Innocenti D, Seyller T, Horn K, and Rotenberg E.
New Journal of Physics 15, 023019 (2013).

Long-lived oscillatory incoherent electron dynamics in molecules: trans-polyacetylene oligomers.
Franco I, Rubio A, and Brumer P.
New Journal of Physics 15, 043004 (2013).

Rashba split surface states in BiTeBr.
Eremeev SV, Rusinov IP, Nechaev IA, and Chulkov, EV.
New Journal of Physics 15, 075015 (2013).

Bulk and surface Rashba splitting in single termination BiTeCl.
Landolt G, Eremeev SV, Tereshchenko OE, Muff S, Slomski B, Kokh KA, Kobayashi M, Schmitt T, Strocov VN, Osterwalder J, Chulkov EV, and Dil JH.
New Journal of Physics 15, 085022 (2013).

Local-field effects on the plasmon dispersion of two-dimensional transition metal dichalcogenides.
Cudazzo P, Gatti M, and Rubio, A.
New Journal of Physics 15, 125005 (2013).

Effect of spin-orbit coupling on atomic-like and delocalized quantum well states in Au overlayers on W(110) and Mo(110).
Shikin AM, Rybkina AA, Rusinova MV, Klimovskikh II, Rybkin AG, Zhizhin EV, Chulkov EV, and Krasovskii EE.
New Journal of Physics 15, 125014 (2013).

Loss spectroscopy of molecular solids: combining experiment and theory.
Roth F, Cudazzo P, Mahns B, Gatti M, Bauer J, Hampel S, Nohr M, Berger H, Knupfer M, and Rubio A.
New Journal of Physics 15, 125024 (2013).

Electronic stopping power of H and He in Al and LiF from first principles.
Zeb MA, Kohanoff J, Sanchez-Portal D, and Artacho E.
Nuclear Instruments and Methods in Physics Research Section B-beam Interactions with Materials and Atoms 303, 59 (2013).

Dynamic screening and energy loss of antiprotons colliding with excited Al clusters.
Koval NE, Sanchez-Portal D, Borisov AG, and Muiño RD.
Nuclear Instruments and Methods in Physics Research Section B-beam Interactions with Materials and Atoms 317, 56 (2013).

Transient metal-like electrical conductivity in swift heavy ion irradiated insulators.
Osmani O, Medvedev N, Juaristi JI, Schleberger M, and Rethfeld B.
Nuclear Instruments and Methods in Physics Research Section B-beam Interactions with Materials and Atoms 317, 72 (2013).

Spectroscopic properties of Er^{3+}-doped fluorotellurite glasses.
Miguel A, Al-Saleh M, Azkargorta J, Morea R, Gonzalo J, Arriandiaga MA, Fernandez J, and Balda R.
Optical Materials 35, 2039 (2013).

Visualizing the near-field coupling and interference of bonding and anti bonding modes in infrared dimer nanoantennas.
Alonso-González P, Albella P, Golmar F, Arzubiaga L, Casanova F, Hueso LH, Aizpurua J, and Hillenbrand R.
Optics Express 21, 1270 (2013).

Optical transport and sensing in plexcitonic nanocavities.
Perez-Gonzalez O, Aizpurua J, and Zabala N.
Optics Express 21, 15847 (2013).

Time-resolved fluorescence line-narrowing of Eu^{3+} in biocompatible eutectic glass-ceramics.
Sola D, Balda R, Al-Saleh M, Pena JI, and Fernandez J.
Optics Express 21, 6561 (2013).

Spectral study of the stimulated emission of Nd^{3+} in fluorotellurite bulk glass.
Miguel A, Azkargorta J, Morea R, Iparraguirre I, Gonzalo J, Fernandez J, and Balda R.
Optics Express 21, 9298 (2013).

Quantum effects and nonlocality in strongly coupled plasmonic nanowire dimers.
Teperik TV, Nordlander P, Aizpurua J, and Borisov AG.
Optics Express, 21, 27306 (2013).

Self-sifting of chain plasmons: the complex optics of Au nanoparticle clusters.
Herrmann LO, Valev VK, Aizpurua J, and Baumberg JJ.
Optics Express 21, 32377 (2013).

On the temporal behavior of Nd^{3+} random lasers.
Iparraguirre I, Azkargorta J, Fernández J, Balda R, García-Revilla S, and Hakmeh N..
Optics Letters 38, 3646 (2013).

Scanning tunneling spectroscopy study of the proximity effect in adisordered two-dimensional metal.
Serrier-Garcia L, Cuevas JC, Cren T, Brun C, Cherkez V, Debontridder F, Fokin D, Bergeret FS, and Roditchev D.
Physical Review Letters 110, 157003 (2013).

Resonant and nonresonant processes in attosecond streaking from metals.
Borisov AG, Sánchez-Portal D, Kazansky AK, and Echenique PM.
Physical Review B 87, 121110(R) (2013).

Sodium molecule on the surface of liquid helium-4 droplets: optical transitions
probe collective excitations.
Tehver I, Hizhnyakov V, and Benedek G.
Physica Status Solidi C 10, 232 (2013)

Initial stage of quasiparticle decay in fermionic systems.
Pavlyukh Y, Berakdar J, and Rubio A.
Physical Review B 87, 125101 (2013).

The natural orbital functional theory of the bonding in Cr_2, Mo_2 and W_2.
Ruiperez F, Piris M, Ugalde JM, and Matxain JM.
Physical Chemistry Chemical Physics : PCCP 15, 2055 (2013).

On the directionality of halogen bonding.
Huber SM, Scanlon JD, Jimenez-Izal E, Ugalde JM, and Infante I.
Physical Chemistry Chemical Physics 15, 10350 (2013).

Quantum chemical study of the catalytic activation of methane by copper oxide and
copper hydroxide cations.
Rezabal E, Ruiperez F, and Ugalde JM.
Physical Chemistry Chemical Physics 15, 1148 (2013).

Resonance-assisted hydrogen bonds revisited. Resonance stabilization vs. charge delocalization.
Góra RW, Majz M, and Grabowski SJ.
Physical Chemistry Chemical Physics 15, 2514 (2013).

Solvent-mediated folding of dicarboxylate dianions:
aliphatic chain length dependence and origin of the IR intensity quenching.
Wanko M, Wende T, Saralegui MM, Jiang L, Rubio A, and Asmis, KR.
Physical Chemistry Chemical Physics 15, 20463 (2013).

Structural, energetic, spectroscopic and QTAIM analyses of cation-pi interactions involving
mono-and bi-cyclic ring fused benzene systems.
Hassan A, Dinadayalane TC, Grabowski SJ, and Leszczynski J.
Physical Chemistry Chemical Physics 15, 20839 (2013).

A DFT/TDDFT study on the optoelectronic properties of the amine-capped
magic $(CdSe)_{13}$ nanocluster.
Azpiroz JM, Matxain JM, Infante I, Lopez X, and Ugalde JM.
Physical chemistry chemical physics: PCCP 15, 10996 (2013).

SAM-like arrangement of thiolated graphene nanoribbons:
decoupling the edge state from the metal substrate.
Cabrera-Sanfelix P, Arnau A, Sanchez-Portal D.
Physical chemistry chemical physics: PCCP 15, 3233 (2013).

Hydrogen and halogen bonds are ruled by the same mechanisms.
Grabowski SJ.
Physical Chemistry Chemical Physics: PCCP 15, 7249 (2013).

Tight-binding models for ultracold atoms in honeycomb optical lattices.
Ibanez-Azpiroz J, Eiguren A, Bergara A, Pettini G, and Modugno M.
Physical Review A 87, 011602 (2013).

Sudden quench in a model Hamiltonian with interactions:
The time-dependent components of Wigner's correlation.
Nagy I.
Physical Review A 87, 052512 (2013).

Phase equilibrium of binary mixtures in mixed dimensions.
Malatsetxebarria E, Marchetti FM, and Cazalilla MA.
Physical Review A 88, 033604 (2013).

Self-consistent tight-binding description of Dirac points moving and merging in
two dimensional optical lattices.
Ibañez-Azpiroz J, Eiguren A, Bergara A, Pettini G, and Modugno M.
Physical Review A 88, 033631 (2013).

Time-dependent exchange-correlation functional for a Hubbard dimer:
Quantifying nonadiabatic effects.
Fuks JI, Farzanehpour M, Tokatly IV, Appel H, Kurth S, and Rubio A.
Physical Review A 88, 062512 (2013).

Dissipative effects on the superfluid-to-insulator transition in mixed-dimensional optical lattices.
Malatsetxebarria E, Cai Z, Schollwock U, and Cazalilla MA.
Physical Review A 88, 063630 (2013).

Origin of chemical contrast in low-energy electron reflectivity of correlated multivalent oxides:
The case of ceria.
Flege JI, Kaemena B, Meyer A, Falta J, Senanayake SD, Sadowski JT, Eithiraj RD, and Krasovskii EE.
Physical Review B 88, 235428 (2013).

Surface and subsurface phonons of Bi(111) measured with helium atom scattering.
Tamtögl A, Kraus P, Mayrhofer-Reinhartshuber M, Campi D, Bernasconi M, Benedek G, and Ernst WE.
Physical Review B 87, 035410 (2013).

Scattering resonances in two-dimensional crystals with application to graphene.
Nazarov VU, Krasovskii EE, and Silkin VM.
Physical Review B 87, 041405 (2013).

Phonons in ultrathin Bi(111) films: Role of spin-orbit coupling in electron-phonon interaction.
Chis V, Benedek G, Echenique PM, and Chulkov EV.
Physical Review B 87, 075412 (2013).

Two-dimensional and pi plasmon spectra in pristine and doped graphene.
Despoja V, Novko D, Dekanic K, Sunjic M, and Marusic L.
Physical Review B 87, 075447 (2013).

Mass enhancement parameter in free-standing ultrathin Pb(111) films:
The effect of spin-orbit coupling.
Sklyadneva IY, Heid R, Bohnen KP, Echenique PM, and Chulkov EV.
Physical Review B 87, 085440 (2013)

Ab initio study of low-energy collective electronic excitations in bulk Pb.
Zubizarreta X, Silkin VM, and Chulkov EV.
Physical Review B 87, 115112 (2013)

Scattering of surface electrons by isolated steps versus periodic step arrays.
Ortega JE, Lobo-Checa J, Peschel G, Schirone S, Abd El-Fattah ZM, Matena M, Schiller F,
Borghetti P, Gambardella P, and Mugarza A.
Physical Review B 87, 115425 (2013).

Evidence for a direct band gap in the topological insulator Bi_2Se_3 from theory and experiment.
Nechaev IA, Hatch RC, Bianchi M, Guan D, Friedrich C, Aguilera I, Mi JL, Iversen BB, Blugel S,
Hofmann P, and Chulkov EV.
Physical Review B 87, 121111 (2013).

Phonon softening and direct to indirect band gap crossover in strained single-layer $MoSe_2$.
Horzum S, Sahin H, Cahangirov S, Cudazzo P, Rubio A, Serin T, and Peeters FM.
Physical Review B 87, 125415 (2013).

Dynamical screening in correlated metals: Spectral properties of $SrVO_3$ in the GW approximation
and beyond.
Gatti M, and Guzzo M.
Physical Review B 87, 155147 (2013).

Grain boundaries with octagonal defects in graphene nanoribbons and nanotubes.
Pelc M, Chico L, Ayuela A, and Jaskolski W.
Physical Review B 87, 165427 (2013).

Natural optical activity and its control by electric field in electrotoroidic systems.
Prosandeev S, Malashevich A, Gui ZG, Louis L, Walter R, Souza I, and Bellaiche L.
Physical Review B 87, 195111 (2013).

Many-body effects on the Rashba-type spin splitting in bulk bismuth tellurohalides.
Rusinov IP, Nechaev IA, Eremeev SV, Friedrich C, Blugel S, and Chulkov EV.
Physical Review B 87, 205103 (2013).

Time evolution of excitations in normal Fermi liquids.
Pavlyukh Y, Rubio A, and Berakdar J.
Physical Review B 87, 205124 (2013).

Resonance-enhanced inelastic He-atom scattering from subsurface optical phonons of Bi(111).
Kraus P, Tamögl A, Mayrhofer-Reinhartshuber M, Benedek G, and Ernst WE.
Physical Review B 87, 245433 (2013).

Phase-dependent heat transport through magnetic Josephson tunnel junctions.
Bergeret FS, and Giazotto F.
Physical Review B 88, 014515 (2013).

Electronic structure of silicene on Ag(111): Strong hybridization effects.
Cahangirov S, Audiffred M, Tang PZ, Iacomino A, Duan WH, Merino G, and Rubio A.
Physical Review B 88, 035432 (2013).

Green's function approach to the lifetimes of image potential resonances at metal surfaces.
Tsirkin SS, Borisov AG, and Chulkov, EV.
Physical Review B 88, 035449 (2013).

Self-consistent GW: All-electron implementation with localized basis functions.
Caruso F, Rinke P, Ren XG, Rubio A, and Scheffler M.
Physical Review B 88, 075105 (2013).

Origin of Rashba splitting in the quantized subbands at the Bi_2Se_3 surface.
Benia HM, Yaresko A, Schnyder AP, Henk J, Lin CT, Kern K, and Ast CR.
Physical Review B 88, 081103 (2013).

Unoccupied topological surface state in Bi_2Te2_2e.
Nurmamat M, Krasovskii EE, Kuroda K, Ye M, Miyamoto K, Nakatake M, Okuda T, Namatame H,
Taniguchi M, Chulkov EV, Kokh KA, Tereshchenko OE, and Kimura A.
Physical Review B 88, 081301 (2013).

Spin-flip transitions and departure from the Rashba model in the Au(111) surface.
Ibanez-Azpiroz J, Bergara A, Sherman EY, and Eiguren A.
Physical Review B 88, 125404 (2013)

$LaAu_2$ and $CeAu_2$ surface intermetallic compounds grown by high-temperature deposition on Au(111).
Ormaza M, Fernandez L, Lafuente S, Corso M, Schiller F, Xu B, Diakhate M, Verstraete MJ, and Ortega JE.
Physical Review B 88, 125405 (2013).

Magnetic proximity effect at the three-dimensional topological insulator/magnetic insulator interface.
Eremeev SV, Men'shov VN, Tugushev VV, Echenique PM, and Chulkov EV.
Physical Review B 88, 144430 (2013).

Exciton dispersion from first principles.
Gatti M, and Sottile F.
Physical Review B 88, 155113 (2013).

Plane-wave based electron tunneling through field emission resonance states.
Garcia-Lekue A, Sanchez-Portal D, Arnau A, and Wang LW.
Physical Review B 88, 155441 (2013).

Visualizing spin-dependent bulk scattering and breakdown of the linear dispersion relation in Bi_2Te_3.
Sessi P, Otrokov MM, Bathon T, Vergniory MG, Tsirkin SS, Kokh KA, Tereshchenko OE, Chulkov EV,and Bode M.
Physical Review B 88, 161407 (2013).

One-dimensional half-metallic interfaces of two-dimensional honeycomb insulators.
Bristowe NC, Stengel M, Littlewood PB, Artacho E, and Pruneda JM.
Physical Review B 88, 161411 (2013).

Quasiparticle band gap in the topological insulator Bi_2Te_3.
Nechaev IA, and Chulkov EV.
Physical Review B 88, 165135 (2013).

Quantum capacitance measurements of electron-hole asymmetry and
next-nearest-neighbor hopping in graphene.
Kretinin A, Yu GL, Jalil R, Cao Y, Withers F, Mishchenko A, Katsnelson MI, Novoselov KS,
Geim AK, and Guinea F.
Physical Review B 88, 165427 (2013).

Theoretical study of the ground-state structures and properties of niobium hydrides under pressure.
Gao GY, Hoffmann R, Ashcroft NW, Liu HY, Bergara A, and Ma YM.
Physical Review B 88, 184104 (2013).

Nonlocal edge state transport in topological insulators.
Protogenov AP, Verbus VA, and Chulkov, EV.
Physical Review B 88, 195431 (2013).

Magnetic proximity effect at the three-dimensional topological insulator/ferromagnetic insulator heterostructure.
Men'shov VN, Tugushev VV, Eremeev SV, Echenique PM, and Chulkov EV.
Physical Review B 88, 224401 (2013).

Time-dependent equation for the magnetic order parameter near the quantum critical point in multiband superconductors with a spin-density wave.
Moor A, Volkov AF, and Efetov KB.
Physical Review B 88, 224513 (2013).

Quasiparticle spectra and excitons of organic molecules deposited on substrates: $G^{(0)}W^{(0)}$-BSE approach applied to benzene on graphene and metallic substrates.
Despoja V, Loncaric I, Mowbray DJ, and Marusic L.
Physical Review B 88, 234437 (2013).

Lattice-matched versus lattice-mismatched models to describe epitaxial monolayer graphene on Ru(0001).
Stradi D, Barja S, Diaz C, Garnica M, Borca B, Hinarejos JJ, Sanchez-Portal D, Alcami M, Arnau A, de Parga ALV, Miranda R, and Martin F.
Physical Review B 88, 245401 (2013).

Knock-on damage in bilayer graphene: Indications for a catalytic pathway.
Zubeltzu J, Chuvilin A, Corsetti F, Zurutuza A, and Artacho E.
Physical Review B 88, 245407 (2013).

Theory of core-level spectra in x-ray photoemission of pristine and doped graphene.
Despoja V, and Sunjic M.
Physical Review B 88, 245416 (2013).

Applicability of mode-coupling theory to polyisobutylene: a molecular dynamics simulation study.
Khairy Y, Alvarez F, Arbe A, and Colmenero J.
Physical Review E 88, 042302 (2013).

Determining the short-range spin correlations in the spin-chain Li_2CuO_2 and $CuGeO_3$ compounds using resonant inelastic x-ray scattering.
Monney C, Bisogni V, Zhou KJ, Kraus R, Strocov VN, Behr G, Malek J, Kuzian R, Drechsler SL, Johnston S, Revcolevschi A, Buchner B, Ronnow HM, van den Brink J, Geck J, and Schmitt T.
Physical Review Letters 110, 087403 (2013).

Effect of nanoconfinement on polymer dynamics: surface layers and interphases.
Krutyeva M, Wischnewski A, Monkenbusch M, Willner L, Maiz J, Mijangos C, Arbe A, Colmenero J, Radulescu A, Holderer O, Ohl M, and Richter D.
Physical Review Letters 110, 108303 (2013).

Singlet-triplet conversion and the long-range proximity effect in superconductor-ferromagnet structures with generic spin dependent fields.
Bergeret FS, and Tokatly IV.
Physical Review Letters 110, 117003 (2013).

Correlated motion of electrons on the Au(111) surface: anomalous acoustic surface-plasmon dispersion and single-particle excitations.
Vattuone L, Smerieri M, Langer T, Tegenkamp C, Pfnür H, Silkin VM, Chulkov EV, Echenique PM, and Rocca M.
Physical Review Letters 110, 127405 (2013).

Comment on "Topological insulators in ternary compounds with a honeycomb lattice".
Vergniory MG, Marques MAL, Botti S, Amsler M, Goedecker S, Chulkov EV, Ernst A, and Romero AH.
Physical Review Letters 110, 129701 (2013).

Bond breaking and bond formation: how electron correlation is captured in many-body perturbation theory and density-functional theory.
Caruso F, Rohr DR, Hellgren M, Ren XG, Rinke P, Rubio A, and Scheffler M.
Physical Review Letters 110, 146403 (2013).

Hybridization of surface waves with organic adlayer librations: a helium atom scatteringand density functional perturbation theory study of methyl-Si(111).
Brown RD, Hund ZM, Campi D, O'Leary LE, Lewis NS, Bernasconi M, Benedek G, and Sibener SJ.
Physical Review Letters 110, 156102 (2013).

Unanticipated proximity behavior in ferromagnet-superconductor heterostructures with controlled magnetic noncollinearity.
Zhu LY, Liu YH, Bergeret FS, Pearson JE, te Velthuis SGE, Bader SD, and Jiang JS.
Physical Review Letters 110, 177001 (2013).

Experimental verification of the spectral shift between near- and far-field peak intensities of plasmonic infrared nanoantennas.
Alonso-González P, Albella P, Neubrech F, Huck C, Chen J, Golmar F, Casanova F, Hueso LE, Pucci A, Aizpurua J, and Hillenbrand R.
Physical Review Letters 110, 203902 (2013).

Robust subnanometric plasmon ruler by rescaling of the nonlocal optical response.
Teperik TV, Nordlander P, Aizpurua J, and Borisov AG.
Physical Review Letters 110, 263901 (2013).

Direct evidence of two equilibration mechanisms in glassy polymers.
Cangialosi D, Boucher VM, Alegria A, and Colmenero, J.
Physical Review Letters 111, 095701 (2013).

Circular dichroism and superdiffusive transport at the surface of BiTeI.
Mauchain J, Ohtsubo Y, Hajlaoui M, Papalazarou E, Marsi M, Taleb-Ibrahimi A, Faure J, Kokh KA, Tereshchenko OE, Eremeev SV, Chulkov EV, and Perfetti L.
Physical Review Letters 111, 126603 (2013).

Experimental evidence of hidden topological surface states in $PbBi_4Te_7$.
Okuda T, Maegawa T, Ye M, Shirai K, Warashina T, Miyamoto K, Kuroda K, Arita M, Aliev ZS, Amiraslanov IR, Babanly MB, Chulkov EV, Eremeev SV, Kimura A, Namatame H, and Taniguchi M.
Physical Review Letters 111, 206803 (2013).

Exact evaluation of entropic quantities in a solvable two-particle model.
Glasser ML and Nagy I.
Physics Letters A 377, 2317 (2013).

Conformal surface plasmons propagating on ultrathin and flexible films.
Shen X, Cui TJ, Martin-Cano D, and Garcia-Vidal FJ.
PNAS (Proceedings of the National Academy of Sciences of the United States of America) 110, 40 (2013).

Local mechanical and dielectric behavior of the interacting polymer layer in silica nano-particles filled SBR by means of AFM-based methods.
Kummali MM, Miccio LA, Schwartz GA, Alegría A, Colmenero J, Otegui J, Petzold A, Westermann S.
Polymer 54, 4980 (2013).

Key ingredients of the alkali atom - metal surface interaction: Chemical bonding versus spectral properties.
Trioni MI, Achilli S, and Chulkov EV.
Progress in Surface Science 88, 160 (2013).

Phonons on the clean metal surfaces and in adsorption structures.
Rusina GG, and Chulkov EV.
Russian Chemical Reviews 82, 483 (2013).

Direct imaging of covalent bond structure in single-molecule chemical reactions.
G. de Oteyza D, Gorman P, Chen Y-C, Wickenburg S, Riss A, Mowbray DJ, Etkin G, Pedramrazi Z, Tsai H-Z, Rubio A, Crommie MF and Fischer FR.
Science 340, 1434 (2013).

Large spin splitting of metallic surface-state bands at adsorbate-modified gold/silicon surfaces.
Bondarenko LV, Gruznev DV, Yakovlev AA, Tupchaya AY, Usachov D, Vilkov O, Fedorov A, Vyalikh DV, Eremeev SV, Chulkov EV, Zotov AV, and Saranin AA.
Scientific Reports 3, 1826 (2013).

Efficient Gate-tunable light-emitting device made of defective boron nitride nanotubes: from ultraviolet to the visible.
Attaccalite C, Wirtz L, Marini A, and Rubio A.
Scientific Reports 3, 2698 (2013).

Octagonal defects at carbon nanotube junctions.
Jaskolski W, Pelc M, Chico L, and Ayuela A.
Scientific World Journal, 658292 (2013).

Confinement of poly(ethylene oxide) in the nanometer-scale pores of resins and carbon nanoparticles.
Barroso-Bujans F, Palomino P, Cerveny S, Fernandez-Alonso F, Rudic S, Alegria A, Colmenero J, and Enciso E.
Soft Matter 9, 10960 (2013).

Fluids of semiflexible ring polymers: effective potentials and clustering.
Bernabei M, Bacova P, Moreno AJ, Narros A, and Likos ChN.
Soft Matter 9, 1287 (2013).

Physical aging in polymers and polymer nanocomposites: recent results and open questions.
Cangialosi D, Boucher VM, Alegria A, and Colmenero J.
Soft Matter 9, 8619 (2013).

Theoretic study of the electronic spectra of neutral and cationic PaO and PaO_2.
Kovacs A, Infante I, and Gagliardi L.
Structural Chemistry 24, 917 (2013).

Valence band electronic structure characterization of the rutile TiO_2 (110)-(1 × 2) reconstructed surface.
Sánchez-Sánchez C, Garnier MG, Aebi P, Blanco-Rey M, de Andrés PL, Martín-Gago JA, and López MF.
Surface Science 608, 92 (2013).

Exploring large O 1s and N 1s core level shifts due to intermolecular hydrogen bond formation in organic molecules.
Garcia-Gil S, Arnau A, and Garcia-Lekue A.
Surface Science 613, 102 (2013).

Surface Debye temperature and vibrational dynamics of Antimony(111) from helium atom scattering measurements.
Tamtogl A, Mayrhofer-Reinhartshuber M, Kraus P, and Ernst WE.
Surface Science 617, 225 (2013).

Vibrational spectroscopy and theory of alkali metal adsorption and co-adsorption on single-crystal surfaces.
Politano A, Chiarello G, Benedek G, Chulkov EV, and Echenique PM.
Surface Science Reports 68, 305 (2013).

Size and branching effects on the fluorescence of benzylic dendrimers possessing one apigenin fluorophore at the core.
Vins P, Vermachova M, Drasar P, del Barrio M, Jarne C, Cebolla VL, de Cozar A, Zangi R, and Cossio FP.
Tetrahedron 69, 10361 (2013).

The one-electron picture in the Piris natural orbital functional 5 (PNOF5).
Piris M, Matxain JM, Lopez X, Ugalde JM.
Theoretical Chemistry Accounts 132, 1298 (2013).

Cooperativity of hydrogen and halogen bond interactions.
Grabowski SJ.
Theoretical Chemistry Accounts 132, 1347 (2013).

Tunable molecular plasmons in polycyclic aromatic hydrocarbons.
Manjavacas A, Marchesin F, Thongrattanasiri S, Koval P, Nordlander P, Sanchez-Portal D, de Abajo FJG.
ACS Nano 7, 3635 (2013)

Fellows Gipuzkoa

Dr. Arantzazu Garcia Lekue
Lawrence Berkeley National Laboratory, USA
01/10/2006–31/10/2012
Electron transport and dynamics in nanostructure materials. Elastic quantum transport through molecular nanodevices, such as molecular based electronic switches. Inelastic effects caused by electronvibration interactions.

Dr. María José Cabrera San Félix
University of Liverpool, United Kingdom and Donostia International Physics Center, Spain
01/11/2007–31/10/2012
Molecular modelling of water ice in atmospheric and astrophysical environments. First-principles calculations of the structural properties and reactivity of water adsorbed, at the monolayer and submonolayer regions, on different surface types: metallic, ionic and graphitic surfaces.

Dr. Thomas Frederiksen
Technical University of Denmark
01/03/2008–14/08/2012
Theory and simulation of electronic transport properties of nanoscale systems. First-principles modeling of current-induced phenomena, inelastic scattering, and local heating. Density functional theory, nonequilibrium Green's functions, electron-phonon coupling, molecular electronics, monatomic chains, fullerenes.

Dr. Laura Férnandez Gómez-Recuero
Technische Universität Dresden, Germany
01/01/2009–31/12/2013
Preparation and characterization of self-assembled metallic nanostructures that reveal magnetic properties. Structural analysis by scanning tunneling microscopy. Magnetic characterization by magnetometry and magneto-optics.

Dr. Maria Blanco Rey
University of Cambridge, United Kingdom
01/12/2010–31/05/2013
Molecular dynamics studies and non-adiabatic effects in the interaction of molecules and atoms with solid surfaces. Inelastic electron scattering. Surface crystallography by low-energy electron diffraction.

Dr. Rubén Esteban Llorente
NIST (National Institute of Standards and Technology), Gaithersburg, Maryland, USA
11/03/2013–Present
Quantum plasmonics.

Dr. Maia García Vergniory
Max Planck Institute of Microstructure Physics, Halle an der Saale, Germany
01/06/2013–Present
Electronic and magnetic properties in ordered and disordered topological insulators.

Dr. Peter Koval
Centro de Física de Materiales CSIC-UPV/EHU, Donostia-San Sebastián, Spain
25/11/2013–Present
Development of MBPT with localized orbitals.

Postdoctoral Positions

Dr. Santiago Rigamonti
Centro Atómico Bariloche, Argentina
23/04/2008–04/05/2012
Electronic structure of low dimensional systems and transport in molecular junctions.

Dr. Marisa Faraggi
Universidad de Buenos Aires, Argentina
05/05/2008–30/04/2012
We study the dynamics of electronic excitation in metallic surfaces focusing on the study of electron-electron and electron-phonon interactions.

Dr. Ludovic Martin-Gronde
Université Bordeaux1, Talence, France
01/09/2009–14/09/2012
Theory of elementary reactive processes at metal surfaces: Calculation of potential energy surfaces from first-principles and evaluation of reaction rates in Eley-Rideal processes.

Dr. Siddhart Surajbhan Gautam
Bhabha Atomic Research Centre, Mumbai, India
04/09/2009–30/09/2012
Structure and dynamics of polymers by neutron scattering and md-simulations.

Dr. Pawel Rejmak
Institute of Catalysis and Surface Chemistry of Polish Academy of Science, Krakov, Poland
02/06/2010–31/05/2013
First-principles calculations on nanostructures.

Dr. Vasse Chis
University of Göteborg, Sweden
15/11/2010–31/12/2012
First-principle calculations of vibrations and electron-phonon interaction in heavy materials.

Dr. Iñigo Garcia Yoldi
Instituto de Ciencia y Tecnología de Polimeros, CSIC Madrid, Spain
01/03/2011–31/08/3012
Simulation of confined polymers.

Dr. Patrizia Borghetti
Universita Cattolica del Sacro Cuore, Brescia, Italy
07/04/2011–30/04/2012
Physical chemistry of interfaces in organic solar cells.

Dr. Alvise Verso
Ulm University, Germany
01/05/2011–31/07/2013
Readout of a superconducting qubit: a problem of quantum escape processes for driven systems.

Dr. Alejandro Miccio
Facultad de Ingeniería - INTEMA, Mar del Plata, Argentina
21/07/2011–14/04/2013
Local Dielectric Spectroscopy by means of AFM.

Dr. Eithiraj Rajagopal Dashinamoorthy
Anna University, India
18/08/2011–31/08/2013
Computational solid state spectroscopy

Dr. Debsindhu Bhowmik
Laboratoire Léon Brillouis (CEA-NRS), Gif-sur-Yvette, France
01/01/2012–18/12/2013
Behavior of hydrophobic ions in aqueous medium.

Dr. Orkhan Osmani
Universität of Duisburg-Essen, Fakultät für Physik, Duisburg ,Germany
09/01/2012–31/12/2012
Nanostructure formation under swift heavy ion irradiation of metals and insulators.

Dr. Andrew Walter
La Trobe University, Australia
06/03/2012–23/07/2013
Electronic structure investigations on defect arrays by angle resolved photoemission.

Dr. Ilya Nechaev
Tomsk State University, Russia
03/04/2012–Present
Electronic structure and many-body effects in layered semiconductors.

Dr. Christos Tserkezis
University of Athens, Greece
01/08/2012–Present
Optical properties of metamaterials.

Dr. Noelia Luque
Universidad Nacional de Córdoba, Argentina
01/11/2012–Present
Ab-initio quantum chemistry studies of seleno-L-cysteine on coinage metal surfaces.

Dr. Stepan Tsirkin
State University of Tomsk, Russia
04/12/2012–Present
Magnetic proximity effect in the layered structures.

Dr. Pablo Aguado Puente
Universidad de Cantabria, Santander, Spain
01/01/2013
Coupling of ferroic nanoscale films with interfacial two dimensional electron gases in oxides.

Dr. Chang-Jin Lee
Boston College, Massachusetts, USA
01/04/2013
Electronic excitations and many-body effects in solids, surfaces, and nanostructures.

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

Dr. Maria de Retamosa Hernandez
Facultad de Química, UPV/EHU, Donostia-San Sebastián, Spain
01/07/2013
Remote structural effects in unnatural amino acids.

Dr. Rubén González Moreno
Instituto de Ciencia de Materiales de Madrid, CSIC, Spain
01/07/2013
Fabrication of curved single crystals.

Dr. Mikhail Otrokov
State University of Tomsk, Russia
17/07/2013
Topological insulators.

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

Temporary Contract Position

Dr. Irina Sklyadneva
Russian Academy of Sciences, Tomsk, Russia
14/05/2003–Present
Surface phonons and electron-phonon interactions in bulk metals and at metal surfaces. Electron-phonon interactions are of paramount importance for the correct description of the temperature dependence of quasiparticle dynamics in bulk metals and at metals surfaces. The goal of the present project is calculations of electron-phonon interactions for overlayers of alkali metals on simple and noble metal surfaces. These calculations will be also done for superconducting materials like MgB2 and for semimetals.

PhD Students

Olalla Pérez González
Facultad de Ciencia y Tecnología, Universidad del País Vasco/Euskal Herriko Unibertsitatea,
Donostia-San Sebastián, Spain
02/10/2006–31/03/2012
Plasmon excitations in metallic nanoparticles. Optical properties of nanostructured materials.

Marco Bernabei
Universita di Roma Tre, Roma, Italy
29/10/2007–31/01/2012
Molecular dynamics simulations of simple models for glass-forming polymers.

Zakaria Mohammed Slimani
Centre Européen de Calcul Atomique et Moléculaire (CECAM), Lyon, France
24/02/2009–23/08/2013
Dynamics of diblock copolymers by computer simulations (Ph.D.) Computer simulations of self-assembly and slow dynamics in diblock copolymers.

Mohamed Ameen Poyli
Bharathidasan University, Tiruchirappalli Tamil Nadu, India
01/06/2010–31/01/2012
Photonic Nanoantennas.

Elixabete Goiri Little
Facultad de Ciencias y Tecnología, Universidad del País Vasco/Euskal Herriko Unibertsitatea, Leioa, Spain
01/07/2010–Present
Tunneling microscopy and spectroscopy of molecules on metals at 1 K.

Mario Lechner
Johannes Kepler Universität Linz, Austria
01/09/2010–31/08/2012
Design and self-assembly of polymer-based nanoparticles by computer simulations.

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

Rubén González Moreno
Instituto de Ciencia de Materiales de Madrid, CSIC, Spain
27/07/2011–30/06/2013
Properties and organization of protoporpyrin IX molecules on metal and oxide surfaces.

Mikolaj Kajetan Schmidt
Copernico University, Torun, Poland
13/10/2011–31/03/2013
Radiative decay of emitters in the presence of magnetic dipoles.

Zakaria Abd El-Fattah
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Centro de Física de Materiales CSIC-UPV/EHU,
Donostia-San Sebastián, Spain
07/05/2012–13/02/2013
Electronic/structure interplay in self-assembled nanostructured noble metal surfaces.

Ali Akbari
Centro de Física de Materiales CSIC-UPV/EHU, Donostia-San Sebastián, Spain
01/07/2012–18/04/2013
Time-dependent reduced density matrix and density functional formalisms for many electron systems.

Itziar Gokoetxea Martinez
Centro de Física de Materiales CSIC-UPV/EHU, Donostia-San Sebastián, Spain
01/07/2012–31/03/2013
Scattering and reactive processes in gas/surface dynamics.

Juan Pablo Echeverry Enciso
Centro de Física de Materiales CSIC-UPV/EHU, Donostia-San Sebastián, Spain
01/07/2012–14/01/2013
Low-energy collective electronic excitations in graphite intercalated compounds.

Peio Garcia Goiricelaya
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Leioa, Spain
01/11/2012–31/01/2013
Electron-phonon interaction and non-adiabatic processes in nano-structures.

Maider Ormaza Saezmiera
Centro de Física de Materiales, CSIC-UPV/EHU, Donostia-San Sebastián, Spain
01/01/2013–30/06/2013
Electronic structure of rare-earth, surface alloys.

Anton Xose Brión 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
Modelling energy exchange in gas/surface interactions by means of ab-initio molecular dynamics.

Aitzol Iturbe Beristain
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Leioa, Spain
01/10/2013–Present
Electron-phonon interaction in surfaces with strong spin-orbit interaction.

Oihana Galparsoro Larraza
Facultad de Quimica, Universidad del País Vasco/Euskal Herriko Unibertsitatea,
Donostia-San Sebastián, Spain
01/10/2013–Present
Phonon and electron excitations in diatom abstraction from metallic surfaces.

Long visits

Dr. José Luis Cabellos
CIO, Centro de Investigaciones en Optica, A.C., México
01/12/2011–30/05/2012
Charge transfer and interactions in donor-acceptor/metal systems.

Phd student Petr Vins
Institute of Chemical Technology ICT, Prague, Czech Republic
09/01–30/05/2012
Synthesis of dendrimers with incorporated fluorescent indole core.

Dr. Galina Rusina
Russian Academy of Sciences, Tomsk, Russia
01/11/2011–28/01/2012, 16/02–15/05/2013
Surface phonons in CuPd surface alloyes.

Dr. Nicolay Zaytsev
Ufa State Aviation Technical University, Ufa, Russia
07/11/2011–04/01/2012
First principle electronic structure calculations of organic molecules absorbed on metallic surfaces.

Dr. Alexey Kuzmenko
Université de Genève, Switzerland
07/11/2011–15/02/2012
Optics of Graphene.

Dr. Stepan Tsirkin
State University of Tomsk, Russia
16/11/2011–13/02/2012
Electronic excitations on metal surfaces, topological insulators.

Prof. Vladimir Menshov
Russian Research Center "Kurchatov Institute", Moscow, Russia
21/07/2010–30/11/2012, 09/01–08/04/2012, 03/04–30/06/2013
Magnetic impurities in digital alloys and topological insulators.

Dr. Andrew Walter
Lawrence Berkeley National Laboratory, USA and Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
26/01–27/02/2012
Electronic Structure of Graphene: Simple but Complex.

Prof. Victor Tugushev
Russian Research Center "Kurchatov Institute", Moscow, Russia
02/02–27/04/2012, 04/09–4/11/2012, 03/04–27/06/2013, 07/10–05/12/2013
Magnetism in superlattices and spintronics.

Dr. Guido Walther
Leibniz Institute for Catalysis, University of Rostock, Germany
27/02–06/04/2012
Methane Oxidation on Gold - Elucidation of a mechanism using micrkinetic modelling.

Phd student Martin Hrtoň
Brno University of Technology, Czech Republic
01/03–07/09/2012
Optical properties of nanoscale systems.

Phd student Marcela Penoff
Universidad Nacional de Mar del Plata, Argentina
02/03–02/04/2012
Hydrophobicity studies by means of atomic force microscopy.

Prof. Roman Kuzian
Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Kiev, Ukraine
05/03–31/05/2012
Resonant inelastic X-ray scattering (RIXS).

Dr. Svetlana Borisova
Physics and Materials Science,
Russian Academy of Sciences, Tomsk, Russia
10/03–09/05/2012, 16/02–15/04/2013
Defects and vibrations in topological insulators.

Prof. Vladimir Nazarov
Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan
18/03–18/04/2012
Time-dependent density-functional theory of particle-solid interactions.

Phd student Kaike Yang
Xiangtan University, China
01/04–30/06/2012
Thermoelectrics.

Prof. Istvan Nagy
Technical University of Budapest, Hungary
30/04–23/06/2012
Various aspects of correlations in extended fermionic systems; spice-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Prof. Anatoly Volkov
Ruhr-Universitaet Bochum, Germany
01/05–22/06/2012
Superconductor-Ferromagnet hybrid structures.

Prof. Juan José Saenz Gutierrez
Universidad Autónoma Madrid, Madrid, Spain
08/05–31/07/2012, 01/06–31/07/2013
Nanophotonics. Modeling scanning probe micro-scopies.

Prof. Wolfgang Schattke
Universität Kiel, Germany
16/05–15/08/2012, 01/10–30/11/2013
Variational Quantum Montecarlo calculations of the electronic properties of solids and surfaces. Theory of photoemission in semiconductors and metals.

Prof. Nikolay Kabachnik
Institut fur Experimentalphysik, Hamburg, Germany
02/06–27/08/2012, 01/07–30/09/2013
Study of Auger processes in gases and at solid surfaces within an attosecond streaking scheme.

Phd student Carlo Motta
Universitá di Milano-Bicocca, Italy
10/06–29/07/2012
Ab-initio study of transport in nanojunctions: application to dye-sensitized solar cells.

Phd student Chen Li
Chinese Academy of Sciences, Beijing, China
16/06–13/09/2012
Quantum effects in plasmonics.

Prof. Francisco J. Garcia Vidal
Facultad de Ciencias,
Universidad Autónoma de Madrid, Spain
30/06–11/08/2012
Plasmonics.

Prof. Andrey Borisov
Université Paris Sud, France
01/07–31/08/2012
Time dependent density functional theory calculations to address the optical response of plasmonic systems.

Prof. Bo Hellsing
University of Gothenburg, Sweden
01/07–31/07/2012, 07/08–30/09/2013
Electron-phonon interactions on metal surfaces.

Dr. Sergey Eremeev
Institute of Strength Physics and Materials Sciences, Tomsk, Russia
14/07–11/10/2012, 15/03–12/06/2013, 20/09–20/12/2013
Electronic properties of topological insulators.

Prof. Ulrich Höfer
Philipps-Universität Marburg, Germany
15/07–15/09/2012
Resonance hopping on surfaces of simple metals.

Phd student Hernan Santos-Exposito
Instituto de Ciencia de Materiales de Madrid (ICMM), Madrid, Spain
16/07–30/09/2012
Graphene nanoribbons.

Dr. Ziya Aliyev
Baku State University, Azerbaijan
25/07–22/09/2012, 04/07–02/09/2013
Materials physics of topological insulators.

Prof. Vladimir Kuznetsov
Tomsk State University, Russia
28/07–29/08/2012, 28/07–28/08/2013
Density functional methods in the theory of phase diagrams of alloys and in the Kondo effects.

Prof. Stefan Maier
Imperial College London, United Kingdom
01/08–07/09/2012
Plasmonics for sensing.

Prof. Amand Lucas
FUNDP, Namur, Belgium
02/08–27/10/2012, 02/09–31/10/2013
Condensed matter physics, surface sciences, electronic and atomic structures of reduced dimensionality systems structural biology.

Dr. Yury Koroteev
Tomsk State University, Russia
20/08/2012–19/09/2012, 19/04–17/06/2013, 24/10–22/12/2013
First principles calculations of electronic structure and quasiparticle lifetimes in metals.

Prof. Pedro Luis de Andres Rodríguez
Instituto Ciencia de Materiales de Madrid, CSIC, Madrid, Spain
01/09–31/10/2012
Effect of stress in the chemical activity of graphene.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Italy
11/09–11/11/2012, 09/09–30/10/2013
Surface phonons and phase transitions.

Dr. Antonio Politano
Università degli Studi della Calabria, Italy
21/09–26/10/2012
Adsorption, electronic properties and collective excitations (phonons, plasmons) in thin metal films and graphen.

Prof. Marijan Sunjic
University of Zagreb, Croatia
23/09–07/11/2012, 03/09–30/10/2013
Dynamical response and surface excitations in thin films.

Dr. Tatiana Menshchikova
State University of Tomsk, Russia
17/10–15/12/2012
Excitations on surfaces with defects.

Phd student Anastasia Riabishchenkova
State University of Tomsk, Russia
25/10–25/11/2012
Topological insulators surfaces.

Dr. Mikhail Otrokov
State University of Tomsk, Russia
26/10–22/12/2012, 14/02–16/03/2013
Electronic structure of the magnetic semiconductor digital alloys.

Prof. Raffaele Resta
Universitá di Trieste, Italy
01/12/2012–28/02/2013
Computational modelling of materials physics.

Phd student Raquel Gonzalez Teresa
Fundación Tecnalia, Bilbao, Spain
03/12/2012–02/03/2013
Structural models of cements.

Phd student Afaf El-Sayed Abd-el-Mottaleb Masoud
University Al-Azar, El Cairo, Egypt
23/12/2012–23/02/2013
Molecular assemblies on metal surfaces.

Dr. Sara Garcia Revilla
ETS Ingenieros Industriales y Telecomunicaciones
UPV/EHU, Bilbao, Spain
01/01–31/05/2013
Modelling of light propagation in inhomogenous (micro-nano) dielectric materials, and study of the random lasing dynamics within organic-inorganic hybrid materials.

Dr. Fernando Ruipérez Cillán
Stockholm University, Sweden
06/01–27/06/2013
Quantum chemical studies of elementary catalytic reactions in the gas phase in transition metal containing systems.

Phd student Patrick Kraus
Istitut für Experimentalphysik Technische Universität Graz, Austria
07/01–29/06/2013
Theory of surface dynamics and electron-phonon interaction of topological insulators, in connection with the inelastic atom scattering experiments.

Prof. Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
01/02–31/07/2013
Nanostructure materials.

Prof. Norman March
University of Antwerpen, Belgium
04/02–08/04/2013
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.

Prof. Alexander Protogenov
Institute of Applied Physics of Russian Academy of Sciences, Nizhnii Novgorod, Russia
16/02–31/03/2013
Transport properties of 3D topological insulators.

Prof. Tomas Neuman
Brno University of Technology, Czech Republic
17/02–16/08/2013
Light-matter interactions in the nanoscale.

Dr. Miguel Angel Cazalilla Gutierrez
CSIC, San Sebastián, Spain
01/04–30/04/2013
Strongly correlated systems, Bose Condensates, mesoscopic and low-dimensional systems in and out of equilibrium. Electronic excitations in surfaces and anisotropic systems.

Prof. John Dobson
School of BPS & Queensland Micro and Nanotechnology Centre, Griffith University, Queensland, Australia
15/04–18/05/2013
Van der Waals dispersion forces and current density functional theory.

Prof. Vladlen Zhukov
Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia.
15/04–13/07/2013
Electron dynamics in oxides: electron-electron and electron-phonon mechanisms of decay of excited electrons.

Phd student Garikoitz Aguirregabiria Achutegui
Universitat Politècnica de Catalunya, BarcelonaTech, Spain
16/04–30/09/2013
Electron dynamics in oxides: electron-electron and electron-phonon mechanisms of decay of excited electrons.

Phd student René Jestädt
Fritz-Haber-Institut der Max-Planck-Gesellschaft and FU-Universitat Berlin, Germany
01/05–31/07/2013
Non adiabatic electron ion dynamics in molecular nanostructures: exact versus TDDFT.

Phd student Simon Philipp Rittmeyer
Technical university of Münich, Germany
05/05–07/06/2013
Electronics excitations for oxygen adsorbed in silver surfaces.

Dr.Alejandro Reyes Coronado
Instituto de Física 'Ing. Luis Rivera Terrazas' de la Benemérita Universidad Autónoma de Puebla, México
05/06–06/07/2013
Optical response of resonant metallic nanostructures in surface-enhanced microscopy and spectroscopy. Forces in metallic particles induced by fast electrons.

Phd student Arturo Santos Gómez
Instituto de Física 'Ing. Luis Rivera Terrazas' de la Benemérita Universidad Autónoma de Puebla, México
05/06–06/07/2013
Plasmonic forces induced by fast electron beams.

Prof. Francisco Guinea Lopez
Inst.Ciencia Materiales de Madrid CSIC, Spain
21/06–21/07/2013
Condensed matter physics.

Prof. Anatoly Volkov
Ruhr-Universität Bochum, Germany
01/07–31/07/2013
Superconductor-Ferromagnet hybrid structures.

Prof. Roman O. Kuzian
Institute for Problems of Materials Science, National Academy of Sciences of Ukraine
01/07–28/09/2013
Response function of strongly correlated systems.

Phd student Giacomo Lovat
Università di Trieste and CNR-IOM, Italy
02/07–02/09/2013
Charge transfer at interfaces for photovoltaic applications.

Prof. Imamaddin Amiraslanov
Institute of Physics, ANAS, Baku, Azerbaijan
03/07–05/08/2013
Thermoelectric materials growth and crystal structures.

Dr. Zakaria Mohammed Abd El-Fattah
Faculty of Science, Al-Azhar University, El Cairo, Egypt
06/07–04/10/2013
Angle resolved photoemission experiments in metallic nanostructures.

Phd student Fulvio Berardi
Politecnico de Milano, Milano, Italy
01/08–31/12/2013
Software development and calculations for linear and nonlinear response functions of nanostructures and extended systems within TDDFT.

Dr. Vito Despoja
University of Zagreb, Croatia
01/08–30/09/2013
Within the present project the investigator use ab-initio TD-DFT approach to investigate the time dependent screening and spectrum of C1s core hole created in graphene in XPS experiment.

Dr. Marisa Faraggi
Instituto de Astronomía y Fisica del Espacio IAFE (CONICET-UBA) Ciudad Autónoma de Buenos Aires, Argentina
20/08–18/10/2013
Study of electronic dynamics on transitions metals dichalcogenides (TMDC) and modelling of 2D metal-organic networks on metallic surfaces.

Phd student Rasmus Chirstensen
DTU Nanotech, Technical University of Denmark, Lyngby, Denmark
16/09–16/10/2013
Inelastic transport in nanoscale systems.

Dr. Bruce Milne
Centre for Computational Physics, University of Coimbra, Coimbra, Portugal
21/10–20/12/2013
Theoretical spectroscopy of the light harvesting complex from green plants.

Prof. Alexander Protogenov
Institute of Applied Physics of Russian Academy of Sciences, Nizhnii Novgorod, Russia
31/10–02/12/2013
Transport properties of 3D topological insulators.

Dr. Marta Pelc
Instituto de Ciencia de Materiales CSIC, Madrid, Spain
17/11–17/12/2013
Graphene and carbon nanotubes.

Short visits

Prof. Lawrence Glasser
Clarkson University, New York, USA
08/01–15/01/2012
Mathematical physics applied to condensed matter.

Prof. Istvan Nagy
Technical University of Budapest, Hungary
03/01–28/01/2012, 26/08–08/09/2012, 20/08–15/09/2013
Various aspects of correlations in extended fermionic systems; spice-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Dr. Patrick S. Kirchmann
Fritz Haber Institute of the Max Planck Society, Berlin, Germany
22/01–25/01/2012
Femtosecond time- and angle-resolved photoemission spectroscopy.

Prof. Otto Muskens
University of Southampton, United Kingdom
23/01–24/01/2012, 21/07–25/07/2013
Nanophotonics and optical nanoantenna.

Prof. Andrey Borisov
Université Paris Sud, France
26/01–28/01/2012, 15/11–30/11/2012
Time dependent density functional theory calculations to address the optical response of plasmonic systems.

Dr. Elisa Palacios Lidon
CIOyN, Universidad de Murcia, Spain
27/01–27/01/2012
Study of the nanoscale surface photovoltage of organic semiconductors combining optical and Kelvin probe microscopy.

Prof. James D. Talman
University of Western Ontario, London, Ontario, Canada
29/01–11/02/2012, 03/10–12/10/2012
Efficient methods in quantum chemistry.

Dr. Arnaud Arbouet
Centre d'Elaboration de Matériaux et d'Etudes Structurales, CNRS/Université Paul Sabatier, Toulouse, France
31/01–01/02/2012
Femtosecond optical spectroscopy of the ultrafast dynamics of metal nanoparticles.

Prof. Marijan Sunjic
University of Zagreb, Croatia
01/02–28/02/2012, 02/04–30/04/2013
Dynamical response and surface excitations in thin films.

Dr. Vito Despoja
University of Zagreb, Croatia
01/02–01/03/2012
Within the present project the investigator use ab-initio TD-DFT approach to investigate the time dependent screening and spectrum of C1s core hole cretated in graphene in XPS experiment.

Prof. Peter Sigmund
University Southern Denmark, Odense, Denmark
09/02–11/02/2012
News on particle penetration: Molecules, wakes and Fermi gas.

Prof. Eugene Kogan
Bar-Ilan University, Ramat-Gan, Israel
12/02–22/02/2012, 14/07–27/07/2013
Electronic properties of graphene.

Prof. David Guéry-Odelin
Université Paul Sabatier, Toulouse, France
16/02–18/02/2012
Guided atom optics: recent progress and applications.

Dr. Federica Lo Verso
Institute of Physics, University of Mainz, Germany
21/02–24/02/2012
Computer simulations of polymers in solution: self-assembly and phase behaviour.

Dr. Javier Gorosabel Urkia
Instituto de Astrofísica de Andalucía, Granada, Spain
23/02–01/03/2012, 01/08–19/08/2013
Astronomical instrumentation: a window of opportunities.

Prof. Vitaly N. Golovach
INAC/SPSMS, CEA Grenoble, France
23/02–25/02/2012, 05/08–8/08/2012
Holes confined in SiGe nanostructures. Semiconductor spintronics.

Dr. Pascal Larregaray
ISM, UMR5255, Université Bordeaux1/CNRS, Talence, France
29/02–02/03/2012
Energy dissipation channels in elementary reactive processes at surfaces.

Prof. Vitali Dugaev
Martin-Luther-Universität Halle-Wittenberg, Germany
01/03–01/03/2012
Anomalous Hall effect in two-dimensional electron system in periodic magnetic field.

Dr. Shiro Kawabata
National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan and LPMMC, Universite Joseph Fourier and CNRS, Grenoble, France
04/03–07/03/2012
Transport theory of ferromagnetic-insulator Josephson junctions.

Prof. Imir Ilyas Aliyev
Institue of Chemical Problems of National Academy of Science of Azerbaijan, Baku, Azerbaijan
21/03–28/03/2012
Growth of topological insulators materials.

Prof. Mahammad Babanly
Baku State University, Azerbaijan
21/03–28/03/2012, 01/12–08/12/2012, 07/12–14/12/2013
Experimental investigations of topological insulators.

Phd student Christos Tserkezis
University of Athens, Greece
22/03–24/03/2012
Optical properties of metamaterials.

Dr. Jason Robinson
University of Cambridge, United Kingdom
18/04–20/04/2012
Spin-polarised supercurrents in artificial magnetic domain walls.

Dr. Martin Svec
Institute of Physics ASCR, Praha, Czech Republic
02/04–03/04/2012, 10/04–14/04/2012
2D novel materials on metals and semiconductors.

Dr. Javier Bermejo
Facultad de Ciencia y Tecnología, UPV/EHU, Leioa, Spain
12/04–12/04/2012
The ESS-Bilbao facility: Baseline design and foreseen applications.

Prof. Ivan P. Chernov
Politechnic University of Tomsk, Russia
16/04–22/04/2012
Dynamics of hydrogen in metals under external irradiation.

Phd student Zakaria Mohammed Abd El-Fattah
Universidad del País Vasco UPV/EHU, Centro de Física de Materiales CFM/CSIC, San Sebastián, Spain
16/04–06/05/2012
Electronic/structure interplay in self-assembled nanostructured noble metal surfaces.

Phd student Avradeep Pal
University of Cambridge, United Kingdom
18/04–20/04/2012
Josephson junctions with ferromagnetic insulators.

Dr. Remi Avriller
CNRS, Université Bordeaux1, France
25/04–28/04/2012
Inelastic quantum transport properties of nanoscale objects.

Prof. Agustin Sanchez Lavega
UPV/EHU, Escuela Ingenieros de Bilbao.
18/04–18/04/2012
Las atmósferas de los planetas: Ciencia básica, aplicada y desarrollo tecnológico.

Prof. Aart W. Kleyn
HIMS, Faculty of Science, University of Amsterdam, Holland
01/05–05/05/2012
Scattering of hyperthermal atoms and molecules from metal surfaces.

Prof. Holger L. Meyerheim
Max-Planck-Institut für Microstrukturphysik, Halle, Germany
05/05–08/05/2012
Topological insulators.

Prof. Miguel Angel Garcia Aranda
Universidad de Malaga, Spain
07/05–08/05/2012
Crystallography of cementitius materials.

Prof. Karsten Reuter
Technische Universität München, Garching, Germany
08/05–11/05/2012
Beat the heat!

Prof. Federico Mayor Zaragoza
President of Foundation Culture of Peace, and former General Director of UNESCO
14/05–14/05/2012
Dare to know and know how to dare.

Dr. Jose Canet Ferrer
Universidad de Valencia, Spain
16/05–18/05/2012
Metamateriales (nanofotonica).

Prof. Ivan Scheblykin
Lund University, Lund, Sweden
19/05–26/05/2012
Single molecule spectroscopy approach to energy migration in individual nanostructures - from conjugated polymers to molecular aggregates.

Dr. Gisela Bocan
Centro Atómico Bariloche, Argentina
20/05–01/06/2012, 12/04–27/04/2013
Gas-surface systems, dynamics of diatomic molecules impinging on metallic surfaces, dissociative adsorption and scattering, exchange-correlation and DFT calculations, potential energy surface calculations.

Prof. Joachim Sauer
Humboldt-Universitaet zu Berlin, Institut fuer Chemie, Berlin, Germany
21/05–23/05/2012
Quatum chemistry: methods for investigating the structure, dynamics and reactivity of large chemical systems.

Prof. Thomas Ferrell
University of Tennessee, Knoxville, USA
23/05–25/05/2012, 18/09–15/10/2012
Condensed matter and surface physics; surface plasmons.

Prof. Jorge E. Valdés Leyton
Laboratorio de Colisiones Atómicas (LCA), Universidad Técnica Federico Santa María, Valparaíso, Chile
27/05–26/06/2012
Proton beam interaction with mono-crystalline solids and carbon nanotubes.

Prof. James Hone
Columbia University, New York, USA
03/06–05/06/2012
Growth of Graphene and boron nitrade nanostructurres.

Dr. Miguel Angel Cazalilla
CFM-CSIC, Donostia-San Sebastián, Spain
05/06–05/06/2012
Kondo chains on metallic surfaces.

Prof. Jon Marcaide Osoro
Universidad de Valencia, Burjassot, Spain
10/06–16/06/2012, 21/01–25/01/2013
Radio astronomy.

Prof. Roald Hoffmann
Cornell University, New York, USA
10/06–13/06/2012
Applied theoretical chemistry and... poetry and philosophy...

Dr. Daniel Rolles
Max Planck Advanced Study Group (CFEL), Hamburg, Germany
11/06–13/06/2012
Photoelectron difraccion in the gas phase.

Prof. Giancarlo Franzese
Facultat de Fisica, Universitat de Barcelona, Spain
14/06–15/06/2012
Issues in nanosafety and nanomedicine.

Prof. Antonio Hernando Grande
Instituto de Magnetismo Aplicado ADIF, and Universidad Complutense de Madrid, Spain
14/06–15/06/2012
Magnetism on gold-thiolate nanoparticles.

Prof. Norman March
University of Antwerpen, Belgium
18/06–18/07/2012
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. Antonio Tejeda Gala
Institut Jean Lamour-CNRS, Synchrotron Soleil, Paris, France
19/06–19/06/2012
Nearly ideal dispersion on graphene onto C-face SiC.

Phd student Marc Barbry
Université de Bordeaux, France
02/07–5/07/2012
Efficient methods for GW calculations with LCAO basis.

Prof. Gernot Frenking
Marburg University, Germany
06/07–06/07/2012
Unusual Chemical Bonds and Reactivities - Connecting Fundamental Research with Application in Synthetic Chemistry.

Dr. Arash Mostofi
Imperial College London, United Kingdom
07/07–14/07/2012
Theory and simulation of materials.

Dr. Jonathan Yates
University of Oxford, United Kingdom
07/07–12/07/2012
Computational solid-state NMR and EELS spectroscopy, theory and applications of Wannier functions.

Prof. Karen Louise Scrivener
EPFL-Lausanne, Switzerland
09/07–11/07/2012
Nanostructures in cements.

Dr. Christof P. Dietrich
Universität Leipzig, Germany
12/07–13/07/2012
Microcavities in ZnO

Dr. Luca Floreano
IOM-CNR, Laboratorio TASC, Trieste, Italy
12/07–15/07/2012
TiO2(110): a flexible playground for thin film growth of aromatic molecules.

Dr. Miztli Yépez
Moving Light and Electrons Group, Universidad Autónoma de Madrid, Spain
16/07–20/07/2012
Conductance of disordered wires.

Dr. Luis S. Froufe Perez
Surface Spectroscopies & Surface Plasmon Photonics Group, Instituto de Estructura de la Materia - CSIC
16/07–20/07/2012
Light transport and emission in complex media.

Dr. Jean Christophe Tremblay
Universität Potsdam, Germany
17/07–20/07/2012
STM Induced vibrational excitations at metallic interfaces.

Prof. Gabriel Cwilich
Yeshiva University, New York, USA
18/07–27/07/2012
Fluorescence and intensity correlations in random media.

Dr. Jose Ignacio Latorre Sentis
Universitat de Barcelona, Spain
23/07–25/07/2012
Theoretical particle physics.

Prof. Zhenchao Dong
Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, China
28/07–03/08/2012
Molecular fluorescence in scanning tunneling microscopy cavities.

Prof. Stephan W. Koch
University of Marburg, Germany
07/08–09/08/2012
Quantum design of semiconductor materials: laser, quantum optics, and THz applications.

Dr. Dana Codruta Marinica
Institut des Sciences Moléculaires d'Orsay, Université Paris Sud, France
13/08–17/08/2012
Nonlinear effects in plasmonics.

Dr. Seymur Cahangirov
Universidad de Bilkent, Turkia
08/08–01/09/2012
Simulation of properties of systems with strong correlations: oxides and transition metals.

Prof. Teun Klapwijk
Delft University of Technology, The Netherlands
28/08–02/09/2012
Superconducting nanohybrids.

Prof. Alberto Galindo Tixaire
Universidad Complutense de Madrid, Spain
02/09–30/09/2012
Quantum information and quantum algorithms. Basic problems in quantum physics. Completion of a two-volume textbook on advanced quantum mechanics, and a textbook on space-time structure.

Dr. Eduard Matito i Gras
Universidad de Girona, Spain
03/09–24/09/2012
Parellelization of Piris natural orbital functional theory.

Prof. Archie Howie
Cavendish Laboratory, University of Cambridge, United Kingdom
04/09–19/09/2012
Theory of valence electron excitations by fast electrons.

Dr. Daniele Stradi
Universidad Autónoma de Madrid, Spain
24/09–28/09/2012
Self-assembly and reactivity on the graphene/Ru [0001] surface.

Prof. Ulrich Höfer
Philipps-Universität Marburg, Germany
26/09–29/09/2012, 21/07–29/07/2013
Resonance hopping on surfaces of simple metals.

Prof. Jens Güdde
Philipps-Universität Marburg, Germany
26/09–29/09/2012
Two-photoemission of topological insulators.

Prof. Frank Wilczek
Massachusetts Institute of Technology, Center for Theoretical Physics, Cambridge, USA
30/09–07/10/2012
Theoretical Physics

Dr. Javier Recio Cortes
Instituto de Magnetismo Aplicado ADIF, and Universidad Complutense de Madrid, Spain
03/10–05/10/2012
Magnetism on gold-thiolate nanoparticles.

Dr. Mathias Ljungberg
Instituto Ciencia de Materiales de Barcelona CSIC, Spain
06/10–10/10/2012
First principles calculations of complex oxides.

Dr. Jan Höcker
Institute of Solid State Physics, University of Bremen, Germany
08/10–12/10/2012
Surface oxidation and oxidation catalysis on metal surfaces.

Dr. Jan Ingo Flege
Institute of Solid State Physics, University of Bremen, Germany
08/10–12/10/2012
Surface oxidation and oxidation catalysis on metal surfaces.

Prof. Wim Briels
University of Twente, Enschede, Holland
14/10–17/10/2012
Transient forces in soft matter systems.

Prof. Christos N. Lykos
Faculty of Physics, University of Vienna, Austria
16/10–19/10/2012
Effective potentials in soft matter systems.

Phd student Iuliia Sokolnitckaia
State University of Tomsk, Russia
17/10–15/11/2012
Topological insulators.

Phd student Viktoriya Bebneva
State University of Tomsk, Russia
17/10–15/11/2012
Topological insulators.

Prof. Juan de la Figuera Bayon
Instituto de Química Física Rocasolano (CSIC), Madrid, Spain
18/10–20/10/2012
Magnetite and the magnetite surface: a low energy electron microscopy study.

Dr. Jörg Meyer
Theoretische Chemie, Universität Tecnnique Munich, Germany
21/10–30/10/2012
Nonadiabatic effects in gas/surface dynamics.

Prof. Walter Thiel
Max Planck Institut für Kohlenforschung, Mulheim, Germany
29/10–31/10/2012
Modeling biological processes with first principles multiscale approaches.

Dr. Paolo Sessi
University of Wurzburg, Germany
30/10–02/11/2012
Topological insulator.

Prof. Matthias Bode
University of Wurzburg, Germany
30/10–02/11/2012
Topological insulator.

Prof. Jan Peter Toennies
Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany
01/11–07/11/2012
Creating metallic nanowires by quantum turbulences in He bulk and droplets.

Prof. Mikhail Vasilevskiy
University of Minho, Braga, Portugal
04/11–09/11/2012
Surface plasmon-polaritons in multilayer nanostructures.

Prof. Mario Trioni
CNR, Universitá di Milano-Bicocca, Italy
04/11–09/11/2012
Electronic and magnetic properties of thin solid film on metals.

Dr. Francisco del Monte
Instituto de Ciencia de Materiales de Madrid CSIC, Spain
09/11–09/11/2012
Sustainable processes for the preparation of electrically conductive hierarchical carbon materials.

Prof. Luca Persichetti
Università di Roma "Tor Vergata" Roma, Italy
18/11–19/11/2012
Effects of elastic field anisotropy on the heteroepitaxial growth of Ge quantum dots on vicinal Si surfaces.

Prof. Pedro A. Serena Domingo
Instituto Ciencia Materiales Madrid ICMM - CSIC, Madrid, Spain
19/11–20/11/2012
Theory and simulation of nanomaterials.

Phd student Igor Rusinov
Tomsk State University, Russia
23/11–20/12/2012
Electronic structure of the magnetic semiconductor digital alloys.

Phd student Igor Silkin
Tomsk State University, Russia
24/11–20/12/2012
The electronic structure of topological insulators.

Prof. Akio Kimura
University of Hiroshima, Japan
08/12–11/12/2012
Topological insulators photoemission measurements.

Dr. Pol Forn Diaz
California Institute of Technology
07/01–09/01/2013
Atom-photon interface with nanostructures.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
08/01–07/02/2013
Surface phonons and phase transitions.

Dr. Alexey Soluyanov
ETH, Institute of Theoretical Physics, Zurich, Switzerland
13/01–18/01/2013
Ab-initio search for topological materials: routine computation of topological invariants.

Prof. Esa Räsänen
Tampere University of Technology, Finland
06/01–11/02/2013
Correlated Electron dynamics in nanostructures.

Dr. Takashi Kumagai
Fritz Haber Institute of the Max Planck Society, Berlin, Germany
16/01–19/01/2013
Visualization of hydrogen-bond dynamics within water-based model systems on a metal surface.

Prof. Salvador Miret-Artés
CSIC, Madrid, Spain
18/01–20/01/2013
Theory of surface difusión.

Phd student Davide Campi
Universitá di Milano-Bicocca, Milano, Italy
21/01–1/2/2013
Surfaces dynamics of topological insulators.

Dr. Michael Ruggenthaler
University of Innsbruck, Austria
27/01–02/02/2013
Fundamentals of time-dependent density functional theory.

Phd student Andrea Trabattoni
Universitá degli Studi di Milano Bicoca, Milano, Italy
31/01–02/02/2013
Ultrafast dynamics in molecules excited by attosecond.

Prof. Francesca Ferlaino
Institut für Experimentalphysik, University of Innsbruck, Austria
31/01–02/02/2013
A Bose-Einstein Condensate of Strongly magnetic atoms.

Dr. Stefano Fabris
SISSA - Trieste, Italy
10/2–13/02/2013
Frist principle simulations of materials for energy conversión.

Dr. Jaume Navarro
Ikerbasque Research Professor UPV/EHU, Facultad de Filosofía, San Sebastián
15/02–15/02/2013
Electrons in the Thomson family: from waves to particles, and back again.

Dr. Remi Avriller
Laboratoire Onde et Matière Aquitaine (LOMA CNRS), Université Bordeaux1, France
17/02–20/02/2013
Inelastic quantum transport properties of nanoscale objects.

Prof. Arnaud Desmedt
Institut des Sciences Moléculaires, Université de Bordeaux I, Bordeaux, France
18/02–19/02/2013
Dynamics of clathrates hydrates.

Dr. Ludovic Martin-Gronde
Institut des Sciences Moléculaires ISM, Université de Bordeaux I, Talence, France
18/02–19/02/2013
Dynamics of clathrates hydrates.

Dr. Mathias Ljungberg
Instituto Ciencia de Materiales de Barcelona CSIC, Spain and Laboratoire Ondes et Matière d'Aquitaine, Université Bordeaux 1, France
18/02–23/02/2013, 25/03–28/03/2013, 12/08–17/08/2013
First principles calculations of complex oxides. Test of new decomposition of Bloch's orbital products.

Dr. Christos Tzoumanekas
National Technical University of Athens, Greece and Dutch Polymer Institute, Holland
04/03–08/03/2013
Modelling and simulation of polymer dynamics.

Prof. Helen Jansson
Chalmers University of Technology, Göteborg, Sweden
04/03–08/03/2013
The building material group at Chalmers - current research and future projects.

Phd student Julen Ibañez Azpiroz
Facultad de Ciencia y Tecnología, UPV/EHU, Leioa, Spain
27/08–31/12/2012, 14/03–14/03/2013
Magnetic excitations in high temperature superconductors trough ab initio calculations.

Prof. Enrique Solano
Ikerbasque Research Professor UPV/EHU, Leioa, Spain
15/03–15/03/2013
Quantum simulations: our quantum theatre for atoms and photons.

Prof. Malcolm Stott
Queen's University, Kingston, Canada
17/03–01/04/2013
2D electron gas.

Dr. Juan Lopez Valentín
Instituto de Ciencia y Tecnologia de Polimeros (CSIC), Madrid, Spain
19/03–21/03/2013
Silica filled rubber compounds.

Prof. Rolf Heid
Karlsruhe Institute of Technology (KIT), Germany
01/04–05/04/2013
Electron phonon interaction in bulk metals and at surfaces.

Prof. Francisco Guinea Lopez
Inst.Ciencia Materiales de Madrid.CSIC, Madrid, Spain
10/04–13/04/2013
Condensed matter physics.

Dr. Bruno Rousseau
Université de Montréal, Canada
12/04–12/04/2013
Efficient computation of GW energy level corrections for molecules described in a plane wave basis.

Prof. Ludo B.F. Juurlink
Leiden Institute of Chemistry, Leiden University, The Netherlands
16/04–18/04/2013
Surface corrugation effects in dissociation dynamics

Dr. Andrea Donarini
Institute of Theoretical Physics,
University of Regensburg, Germany
21/04–23/04/2013
Transport characteristics of complex interacting nano-junctions.

Prof. John Pendry
Imperial College London, United Kingdom
21/04–23/04/2013, 24/09–04/10/2013
Metamaterials.

Dr. Sebastian Stepanow
Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
24/04–26/04/2013
Physical chemistry of surface-confined metal-organic complexes.

Dr. Ion Errea Lope
Institut de Minéralogie et de Physique de Milieux Condensés, Université Pierre et Marie Curie, Paris, France
26/04–03/05/2013
Anharmonic free energies and phonon dispersions from the self-consistent harmonic approximation.

Prof. Michel A. Van Hove
Institute of Computational and Theoretical Studies (ICTS) Hong Kong Baptist University, Hong Kong
28/04–30/04/2013
Adsorption structures of large molecules on single-crystal metal surfaces.

Prof. Carmen Ocal
ICMAB-CSIC, Barcelona, Spain
06/05–06/05/2013
Atomic force microscopy and scanning tunneling microscopy.

Prof. Jorge Iribas Cerdá
ICMM-CSIC, Madrid, Spain
06/05–06/05/2013
Quantum theory of electronic transport.

Prof. Luisa E. Bausa López
Universidad Autónoma de Madrid UAM, Madrid, Spain
06/05–06/05/2013
Laser physics.

Prof. Marian Paluch
Institute of Physics, University of Silesia, Poland
20/05–22/05/2013
Tutorial on Broadband dielectric spectroscopy as a powerful tool for investigating molecular dynamics and proton reaction kinetics of condensed matter systems at ambient and elevated pressure.

Dr. Sampsa Riikonen
Helsinki University of Technology, Finland
27/05–13/06/2013
Theoretical studies of complex surface recontructions.

Prof. Surendra P. Shah
Northwestern University, Evanston, USA
27/05–01/06/2013
Nanoadditions in cements.

Prof. Luca Tagliacozzo
Instituto de Ciencias Fotónicas, Barcelona
30/05–31/05/2013
Synergies between new tools for studying strongly correlated many body quantum systems.

Prof. Chris Exley
Birchall Centre, Keele University, United Kingdom
03/06–06/06/2013
Aluminum Interactions with Biological systems

Prof. Dominique Costa
Laboratoire de Physico-Chimie des Surfaces, ENSCP Chimie ParisTech, Paris, France
03/06–05/06/2013
Computational Simulations of superoxide absorption in Boehmite.

Dr. Elena Formoso Estensoro
Università della Svizzera Italiana, Lugano, Switzerland
06/06–16/06/2013
Study of aluminum reactive oxygen species.

Dr. Dietrich Foerster
CPMOH/LOMA Université de Bordeaux, France
11/06–14/06/2013, 01/07–04/07/2013, 22/07–27/07/2013
Test of new decomposition of Bloch's orbital products.

Dr. Javier Villegas Hernandez
Unité Mixte de Physique CNRS/Thales, Palaiseau, France
13/06–15/06/2013
Superconductor/ferroic hybrids.

Prof. Talat S. Rahman
University of Central Florida, Orlando, USA
16/06–24/06/2013
Characteristics of functional nanomaterials: insights from first principles.

Prof. Annemarie Pucci
University of Heidelberg,
Kirchhoff Institute for Physics, Germany
19/06–21/06/2013
Field-enhanced infrared spectroscopy.

Dr. Daniel Niesner
University of Erlangen
19/06–23/06/2013
Two-photon photoemission studies of graphene and topological insulators.

Dr. Richard Korytár
Karlsruhe Institute of Technology (KIT),
Institute of Nanotechnology,
Eggenstein-Leopoldshafen, Germany
19/06–21/06/2013
Correlated transport in nanostructures.

Prof. Rémi Carminati
Institut Langevin, ESPCI ParisTech, Paris, France
23/06–28/06/2013
Light scattering in random media.

Dr. Juraj Feilhaver
Universidad Autonoma de Madrid
30/06–05/07/2013
Waves in disordered media.

Dr. Laura Rósales Zárate
Universidad Autonoma de Madrid, Spain
30/06–12/07/2013
Plamonics and nanophotonics.

Dr. Miztli Yepez
Universidad Autonoma de Madrid, Spain
30/06–12/07/2013
Waves in disordered media.

Phd student Hector Ochoa de Eguileor
Instituto Ciencia de Materiales de Madrid, CSIC, Madrid, Spain
01/07–12/07/2013
Graphene theory and models.

Prof. Andrey Borisov
Université Paris Sud, France
04/07–31/07/2013
Time dependent density functional theory calculations to address the optical response of plasmonic systems.

Prof. Salvador Ferrer Fabregas
Synchrotron ALBA, Cerdanyola del Valles, Spain
10/07–14/07/2013
The Alba light source. Present status and perspectives.

Prof. Guido Fratesi
Universidad degli Studi di Milano-Bicocca, Milano, Italy
15/07–18/07/2013
Charge transfer times of adsorbates: dye molecules on TiO2 from first-principles DFT calculations.

Phd student Daniel Traviss
University of Southampton, United Kingdom
16/07–26/07/2013
Nanophotonics and optical nanoantennas.

Dr. Martin Reiris Ithurralde
Max Planck Institute for Gravitational Physics, Golm, Germany
17/07–20/07/2013
A theoretical perspective of black-holes: past and present.

Phd student Tomas Alonso Lanza
Universidad de Cantabria, Santander, Spain
18/07–18/07/2013
Cobalt clusters in nanotubes.

Phd student Adam Stepniewski
Jerry Haber Institute of Catalysis and Surface Chemistry of Poland Academy of Sciences, Krakow, Poland
22/07–27/07/2013
Electronic properties of heterogenous catalysis.

Prof. Ewa Broclawik
Jagiellonian University, Faculty of Chemistry, Krakow, Poland
22/07–27/07/2013
Electronic properties of heterogenous catalysis.

Dr. Fredrik Hage
STFC Daresbury Laboratories, Warrington, United Kingdom
23/07–26/07/2013
Topologically induced confinement and possible negative refraction index in polycrystalline graphene nano-cones by momentum transfer dependent STEM-VEELS.

Prof. Stefan Maier
Imperial College London, United Kingdom
01/08–06/08/2013
Plasmonics for sensing

Dr. Anna Isaeva
Technical University, Dresden, Germany
02/08–11/08/2013
Growth of complex semiconductor structures

Phd student Daniele Stradi
Universidad Autónoma de Madrid (UAM) and IMDEA-Nanoscience, Spain
04/08–06/08/2013
Transport properties of graphene@Ru(0001).

Prof. Nikolaos Stefanou
National and Kapodistrian University of Athens, Greece
06/08–08/08/2013
Light scattering in nanostructures.

Dr. Antonio Politano
Università degli Studi della Calabria, Italy
18/08–30/08/2013
Adsorption, electronic properties and collective excitations (phonons, plasmons) in thin metal films and graphen.

Prof. Wlodzimierz Jaskólski
Institute of Physics Nicholas Copernicus University, Poland
25/08–24/09/2013
Study of quantum dot arrays and nanotube superlattices.

Prof. Herbert Pfnür
Leibniz Universität Hannover, Germany
02/09–04/09/2013
Plasmons in low-dimensional systems.

Prof. Guy Le Lay
CINaM, Aix-Marseille University, Marseille, France and CNR-ISM, Rome, Italy
9/09–11/09/2013
Structural and electronic properties of silicene and germane: synthesis, STM and photoelectron spectroscopy.

Prof. Garnett Bryant
NIST, Gaithersburg, Maryland, USA
14/09–21/09/2013
Nanophotonics.

Prof. Markus Hennrich
Institute for Experimental Physics, University of Innsbruck, Austria
15/09–18/09/2013
Quantum optics and spectroscopy.

Prof. Shangjr Gwo
National Tsing-Hua University, Taiwan
15/09–17/09/2013
Plasmonic nanolasers and nanostructures.

Dr. Leonor Chico Gómez
Instituto de Ciencia de Materiales de Madrid (ICMM), Spain
16/09–21/09/2013
Electronic structure calculations in nanotubes.

Prof. Archie Howie
Cavendish Laboratory, Cambridge, United Kingdom
19/09–5-10/2013
Theory of valence electron excitations by fast electrons.

Dr. Igor Popov
School of Physics, Trinity College Dublin, Ireland
25/09–28/09/2013
Theory of electron transport at the nanoscale.

Phd student Ivor Loncaric
Centro de Física de Materiales CSIC-UPV/EHU San Sebastian, Spain
25/09–25/10/2013
Dissociation dynamics and hot atom diffusion in the interaction of O2
molecules with the Ag(110)surface.

Prof. Aaron Ciechanover
Institute for Research in Medical Sciences at the Technion (Israel Institute of Technology), Haifa, Israel
27/09–04-10/2013
Scientific communication.

Prof. Dudley Herschbach
Harvard University, Massachusetts, USA
27/09–06/10/2013
Scientific communication.

Prof. Davide Donadio
MPI for Polymer Research, Mainz, Germany
28/09–11/10/2013
Theory of nanostructures and transport.

Prof. Juan Ignacio Cirac
Max-Planck-Institut für Quantenoptik, Garching, Germany
28/09–4/10/2013
Scientific communication.

Dr. Mads Engelund
DTU, Copenhagen, Denmark
29/09–5/10/2013
Quantum electron transport in nanosystems.

Prof. Claude Cohen-Tannoudji
Laboratoire Kastler Brossel, París, France
30/09–04/10/2013
Scientific communication.

Prof. Jean Marie Lehn
1987 Nobel Prize in Chemistry
30/09–4/10/2013
Scientific communication.

Dr. Maria Silvia Gravielle
Instituto de Astronomía y Física del Espacio, Universidad de Buenos Aires, Argentina
30/09–10/10/2013
Electron emission from metal surfaces.
Energy loss in fast atom diffraction.

Prof. Rafael Yuste
Columbia University, Biological Sciences, New York, USA
30/09–3/10/2013
Scientific communication.

Prof. John Inglesfield
University of Wales Cardiff, United Kingdom
03/10–31/10/2013
Embedding in photonics and plasmon bands in metallic nanostructures.

Prof. Daniel Farias Tejerina
Universidad Autónoma de Madrid, Spain
15/10–17/10/2013
Phonon dynamics of graphene.

Prof. Roland Pellenq
MIT, Massachusetts, USA
20/10–22/10/2013
Modelling of cements.

Dr. Martin Gradhand
University of Bristol, United Kingdom
27/10–2/11/2013
Spin dependent electronic transport.

Dr. Tatiana Menshchikova
State University of Tomsk, Russia
31/10–28/11/2013
Excitations on surfaces with defects.

Prof. Gilberto Teobaldi
University of Liverpool, United Kingdom
06/11–10/11/2013
Linear-scaling approaches to charge- and energy-transfer in (extended) photo-electro-chemical interfaces.

Dr. Mads Engelund
DTU, Copenhagen, Denmark
07/11–15/11/2013
Modeling of electron transport at the nanoscale.

Prof. Denis Vyalikh
Dresden University of Technology, Dresden, Germany
13/11–15/11/2013
Photoemission measurements of magnetic surface status.

Prof. Kart Kummer
European Sincotron Radiation Facility, Grenoble, France
13/11–15/11/2013
Photoemission measurements of magnetic surface status.

Prof. Nicolas Lorente
Centro de Investigación en Nanociencia y Nanotecnología (CIN2-CSIC), Bellaterra, Spain
14/11–15/11/2013
Inelastic electron tunnelling spectroscopy.

Dr. Adrian Stan
Détaché à Laboratoire des Solides Irradiés, École Polytechnique, Palaiseau, France
17/11–20/11/2013
Many body perturbation theory and electron-electron interactions in transport theory.

Dr. Manuela Garnica Alonso
IMDEA Nanociencia, Madrid, Spain
21/11–22/11/2013
Electron Acceptor Molecules deposited on epitaxial graphene studied by means of Low temperature scanning tunneling microscopy/spectroscopy.

Prof. Peter Apell
Chalmers University of Technology, Goteborg, Sweden
25/11–30/11/2013
Optical response in nanostructures.

Dr. Jan Honolka
Institute of Physics, Academy of Sciences of the Czech Republic (ASCR), Prague, Czech Republic
03/12–06/12/2013
X-ray spectroscopy of 3d magnetic impurities on graphene and graphite: from strong to weak interaction.

Dr. Ioannis Zegkinoglou
University of Wisconsin and Lawrence Berkeley National Laboratory, USA
11/12–14/12/2013
Surface chemistry in organic solar cells.

Ikerbasque Research Fellows

Prof. Richard O. Prum
Yale University, Peabody Museum of Natural History, New Haven, USA
01/09/2011–31/05/2012
Optical properties of natural structures: an evolutionist approach.

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

Prof. Andrey Kazanskiy
University of San Petersburg, Russia
01/01/2012
Investigation of subfemto atto second processes in gases and solids caused by ultrashort laser pulses. Investigation of dynamics of electrons in suface and image states of noble metal and their interaction with adsorbates.

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

Prof. Mario Piris Silveira
University of Eralngen, Nüremberg, Germany
01/01/2012
Energy functional method development. Computational modelling of semiconductor nanocluster and molecular solid phases and polymorfism.

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

Prof. Vyacheslav Silkin
Russian Academy of Science, Tomsk, Russia
01/01/2012
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. Jeremy Baumberg
Cavendish Laboratory, Cambridge, United Kingdom
03/04–30/09/2012
Nanophotonics, optical nanoantennas, plasmonics, field enhanced spactroscopy, sers, seira, optics of tunneling configurations, plasmon excitations in stem, quantum dots, hybrid systems, near field optical microscopy, optoelectronics, quantum optics.

Prof. Thomas Frederiksen
Technical University of Denmark, Denmark
15/08/2012
Quantum transport theory and electronic structure methods.

Prof. Arantzazu Garcia Lekue
Lawrence Berkeley National Laboratory, USA
01/11/2012–30/10/2017
Modeling electron transport at the nanoscale. Theoretical investigation of electron processes at nanostructured surface.

Prof. María José Cabrera San Félix
University of Liverpool, United Kingdom and Fundación Donostia International Physics Center, Donostia-San Sebastián, Spain
01/11/2012–31/10/2017
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.

Prof. Juan José Saenz Gutierrez
Universidad Autónoma de Madrid, Spain
01/09/2013–31/08/2014
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.

Development and applications of time-dependent density matrix functional theory
Ali Akbari (UPV/EHU)
September 2012
Supervisor: Angel Rubio Secades

Tetrapyrrole molecules on metallic and oxide surface: reactivity and structure
Rubén Gonzalez Moreno (Universidad Autónoma de Madrid)
October 2012
Directora: Celia Rogero

Surface states manipulation via surface/interface defects and adsorbates
Zakaria Mohammed Abd El-Fattah (UPV/EHU)
October 2012
Supervisor: Enrique Ortega Conejero

Collective electronic excitations in layered metallic systems
Juan Pablo Echeverry (UPV/EHU)
November 2012
Supervisors: Eugene Tchulkov and Viacheslav Silkin

Reactivity and dynamics of N2 and O2 on different metal surfaces
Itziar Goikoetxea Martínez
February 2013
Supervisors: Maite Alducin and Iñaki Juaristi

Rare earth/Noble metal surface alloys
Maider Ormaza Saezmiera
June 2013
Supervisor: Enrique Ortega Conejero

Slow dynamics in nanostructured phases of diblock, gradient and random copolymers
Mohammed Zakaria Slimani
July 2013
Supervisor: Angel José Moreno Segurado

23/01/2012
Ultrafast photonics with semiconductor nanowires and plasmonic nanoantennas.
Dr. Otto Muskens, University of Southampton, United Kingdom

25/01/2012
Femtosecond time- and angle-resolved photoemission spectroscopy.
Dr. Patrick S. Kirchmann, Fritz Haber Institute of the Max Planck Society, Berlin, Germany

27/01/2012
Study of the nanoscale surface photovoltage of organic semiconductors combining optical and Kelvin probe microscopy.
Dr. Elisa Palacios Lidon, CIOyN, Universidad de Murcia, Spain

01/02/2012
Femtosecond optical spectroscopy of the ultrafast dynamics of metal nanoparticles.
Dr. Arnaud Arbouet
Centre d'Elaboration de Matériaux et d'Etudes Structurales, CNRS/Université Paul Sabatier, Toulouse, France

10/02/2012
News on particle penetration: Molecules, wakes and Fermi gas.
Prof. Peter Sigmund, University of Southern Denmark, Odense, Denmark

13/02/2012
Magneto-plasmonics of graphene.
Dr. Alexey Kuzmenko, Université de Genève, Switzerland

16/02/2012
Electronic structure of graphene.
Prof. Eugene Kogan, Bar-Ilan University, Ramat-Gan, Israel

17/02/2012
Guided atom optics: recent progress and applications.
Prof. David Guéry-Odelin, Université Paul Sabatier, Toulouse, France

24/02/2012
Holes confined in SiGe nanostructures.
Dr. Vitaliy N. Golovach, CNRS Grenoble, France

29/02/2012
Astronomical instrumentation: a window of opportunities.
Dr. Javier Gorosabel Urkia
Instituto de Astrofísica de Andalucía, Granada, Spain

01/03/2012
Anomalous Hall effect in two-dimensional electron system in periodic magnetic field.
Prof. Vitali Dugaev
Martin-Luther-Universität Halle-Wittenberg, Germany

06/03/2012
Manipulation of hyrogen distribution in Pd by injection of ballistic electron.
Dr. Maria Blanco Rey
University of Cambridge, United Kingdom

06/03/2012
Transport theory of ferromagnetic-insulator Josephson junctions.
Dr. Shiro Kawabata
National Institute of Advanced Industrial Science and Technology AIST), Tsukuba, Japan and LPMMC,
Université Joseph Fourier and CNRS, Grenoble, France

23/03/2012
Internal seminar at Nanophotonics Group
PhD Student Christos Tserkezis, University of Athens, Greece

02/04/2012
Theory of Photoemission from crystals.
Prof. Eugene Krasovskii, Universität Kiel, Germany

12/04/2012
The ESS-Bilbao facility: Baseline design and foreseen applications.
Prof. Javier Bermejo, Facultad de Ciencia y Tecnlogía, UPV/EHU, Leioa, Spain

18/04/2012
Las atmósferas de los planetas: Ciencia básica, aplicada y desarrollo tecnológico.
Prof. Agustin Sanchez Lavega, UPV/EHU, Escuela Ingenieros de Bilbao

19/04/2012
Spin-polarised supercurrents in artificial magnetic domain walls.
Dr. Jason Robinson, University of Cambridge, United Kingdom

08/05/2012
Cement research at University of Malaga
Prof. Miguel Angel Garcia Aranda, Universidad de Malaga, Spain

10/05/2012
Beat the heat!
Prof. Karsten Reuter, Technische Universität München, Garching, Germany

14/05/2012
Dare to know and know how to dare.
Prof. Federico Mayor Zaragoza, President of Foundation Culture of Peace and
Former General Director of UNESCO

14/05/2012
Natural orbital functional theory of the molecular electronic structure.
Prof. Mario Piris Silveira, University of Erlangen, Nüremberg, Germany

22/05/2012
Storage and activation of methane – ab initio approach.
Prof. Joachim Sauer
Humboldt-Universitaet zu Berlin, Institut fuer Chemie, Berlin, Germany

23/05/2012
Single molecule spectroscopy approach to energy migration in individual nanostructures –
from conjugated polymers to molecular aggregates.
Prof. Ivan Scheblykin, Lund University, Sweden

05/06/2012
Kondo chains on metallic surfaces.
Dr. Miguel Angel Cazalilla, CFM-CSIC, Donostia-San Sebastián, Spain

11/06/2012
The chemical and physical imagination at work in very tight places' & encounter with young
(and not so young) researchers.
Prof. Roald Hoffmann, Cornell University, New York, USA

13/06/2012
Watching chemistry in action: probing ultrafast chemical dynamics by
time-resolved photoelectron diffraction.
Dr. Daniel Rolles, Max Planck Advanced Study Group (CFEL), Hamburg, Germany

15/06/2012
Issues in nanosafety and nanomedicine.
Prof. Giancarlo Franzese, Facultat de Fisica, Universitat de Barcelona, Spain

15/06/2012
Magnetic fields induced by the human brain activity: the inverse problem.
Prof. Antonio Hernando Grande, Instituto de Magnetismo Aplicado ADIF,
and Universidad Complutense de Madrid, Spain

19/06/2012
Nearly ideal dispersion on graphene onto C-face SiC.
Dr. Antonio Tejeda Gala, Institut Jean Lamour-CNRS, Synchrotron Soleil, Paris, France

06/07/2012
Unusual Chemical Bonds and Reactivities –
Connecting Fundamental Research with Application in Synthetic Chemistry
Prof. Gernot Frenking, University of Marburg, Germany

09/07/2012
First principles prediction of solid-state NMR parameters.
Dr. Jonathan Yates, University of Oxford, United Kingdom

10/07/2012
Microstructural characterisation of calcium silicate hydrates: crystalline and amorphous products.
Prof. Karen Louise Scrivener, EPFL-Lausanne, Switzerland

13/07/2012
Strong correlations and dispersion interactions with non-orthogonal local orbitals.
Dr. Arash Mostofi, Imperial College London, United Kingdom

13/07/2012
TiO2(110): a flexible playground for thin film growth of aromatic molecules.
Dr. Luca Floreano, IOM-CNR, Laboratorio TASC, Trieste, Italy

17/07/2012
A Gutzwiller study of correlated multi-orbital systems.
Prof. Bo Hellsing, University of Gothenburg, Sweden

23/07/2012
The higgs and the soul of science.
Prof. Jose Ignacio Latorre Sentis, Universitat de Barcelona, Spain

07/08/2012
Light-matter interaction mediated by surface plasmons
Prof. Francisco J. Garcia Vidal, Facultad de Ciencias, Universidad Autónoma de Madrid, Spain

08/08/2012
Quantum design of semiconductor materials: laser, quantum optics, and THz applications.
Prof. Stephan W. Koch, University of Marburg, Germany

02/10/2012
Physical philosophy: unexpected intersections.
Prof. Frank Wilczek, MIT Massachusetts Institute of Technology Center for Theoretical Physics, Massachusetts, USA

18/10/2012
Hierarchical self-assembly of associating soft patchy particles.
Prof. Christos N. Lykos, Faculty of Physics, University of Vienna, Austria

19/10/2012
Magnetite and the magnetite surface: a low energy electron microscopy study.
Prof. Juan de la Figuera Bayon, Instituto de Química Física Rocasolano (CSIC), Madrid

30/10/2012
Theoretical studies of enzymatic reactions.
Prof. Walter Thiel, Max Planck Institut für Kohlenforschung, Mulheim, Germany

02/11/2012
Functional hybrid structures of semiconductor nanocrystals.
Prof. Andrey Rogach, Centre for Functional Photonics (CFP), City University of Hong Kong

06/11/2012
Quantum vortices metallic nanowires, and odd spectra in hellium droplets.
Prof. Jan Peter Toennies, Max-Planck Institut für Dynamik und Selbstorganisation, Göttingen, Germany

06/11/2012
Surface plasmon-polaritons in multilayer nanostructures.
Prof. Mikhail Vasilevskiy, University of Minho, Braga, Portugal

09/11/2012
Sustainable processes for the preparation of electrically conductive hierarchical carbon materials.
Dr. Francisco del Monte, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain

13/11/2012
Modeling electron transport at the nanoscale using plane waves.
Dr. Arantzazu Garcia Lekue, Lawrence Berkeley National Laboratory, USA

19/11/2012
Effects of elastic field anisotropy on the heteroepitaxial growth of Ge quantum dots on vicinal Si surfaces.
Prof. Luca Persichetti, Università di Roma "Tor Vergata" Roma, Italy

14/12/2012
Topological order in electronic wavefunctions.
Prof. Raffaele Resta, Universitá di Trieste, Italy

08/01/2013
Atom-photon interface with nanostructures.
Dr. Pol Forn Diaz, California Institute of Technology, USA

10/01/2013
X-ray laser sources for nanotechnology and imaging applications.
Dr. Eduardo Granados Mateo, Massachusetts Institute of Technology (MIT), Cambridge, Massachusetts, USA

16/01/2013
Ab initio search for topological materials: routine computation of topological invariants.
Dr. Alexey Soluyanov, ETH, Institute for Theoretical Physics, Zurich, Switzerland

18/01/2013
Visualization of hydrogen-bond dynamics within water-based model systems on a metal surface.
Dr. Takashi Kumagai, Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany

01/02/2013
Ultrafast dynamics in molecules excited by attosecond XUV pulses.
PhD student Andrea Trabattoni, Universitá degli Studi di Milano Bicoca, Milano, Italy

01/02/2013
A Bose-Einstein Condensate of Strongly magnetic atoms.
Prof. Francesca Ferlaino
Institut für Experimentalphysik, Universität Innsbruck, Austria

22/02/2013
A new family of star-like icosahedral structures for small cobalt clusters.
Prof. Faustino Aguilera Granja, UASLP, Universidad Autónoma San Luis Potosí, México

26/02/2013
The polarization of solids – A Historical perspective.
Prof. Raffaele Resta, Universitá di Trieste, Italy

05/03/2013
The building material group at Chalmers – current research and future projects.
Prof. Helen Jansson, Chalmers University of Technology, Göteborg, Sweden

08/03/2013
Molecular modelling of cavitation in model polyethylene networks.
Dr. Christos Tzoumanekas,
National Technical University of Athens, Greece and Dutch Polymer Institute, Holland

14/03/2013
Spin-flip absorption rate in surfaces with strong spin-orbit interaction.
Doctorand Julen Ibañez Azpiroz, Facultad de Ciencia y Tecnología, UPV/EHU, Leioa, Spain

11/04/2013
Graphene and its unique properties.
Prof. Francisco Guinea Lopez, Instituto de Ciencia Materiales de Madrid CSIC, Spain

12/04/2013
Efficient computation of GW energy level corrections for molecules described in a plane wave basis.
Dr. Bruno Rousseau, Université de Montréal, Canada

17/04/2013
Surface corrugation effects in dissociation dynamics.
Prof. Ludo B.F. Juurlink, Leiden Institute of Chemistry, Leiden University, The Netherlands

22/04/2013
Transformation optics shapes metamaterials.
Prof. John Pendry, Imperial College London, United Kingdom

25/04/2013
Physical chemistry of surface-confined metal-organic complexes.
Dr. Sebastian Stepanow, Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

30/04/2013
Adsorption structures of large molecules on single-crystal metal surfaces.
Prof. Michel A. Van Hove, Institute of Computational and Theoretical Studies (ICTS)
Hong Kong Baptist University, Hong Kong

03/05/2013
Anharmonic free energies and phonon dispersions from the self-consistent harmonic approximation.
Dr. Ion Errea Lope, Institut de Minéralogie et de Physique de Milieux Condensés,
Université Pierre et Marie Curie, Paris, France

21/05/2013
Tutorial on Broadband dielectric spectroscopy as a powerful tool for investigating molecular dynamics and proton reaction kinetics of condensed matter systems at ambient and elevated pressure.
Prof. Marian Paluch, Institute of Physics, University of Silesia, Poland

31/05/2013
Synergies between new tools for studying strongly correlated many body quantum systems.
Prof. Luca Tagliacozzo, ICFO, Instituto de Ciencias Fotónicas, Castelldefels, Barcelona, Spain

12/06/2013
Ionization of nitric acid in ice surface defects.
Dr. Sampsa Riikonen, Helsinki University of Technology, Finland

14/06/2013
Superconductor/ferroic hybrids.
Dr. Javier Villegas Hernandez, Unité Mixte de Physique CNRS/Thales, Palaiseau, France

20/06/2013
Manipulation of electronic and chemical properties of single layer MoS2: insights from ab initio calculations.
Prof. Talat S. Rahman, University of Central Florida, Orlando, USA

21/06/2013
Two-photon photoemission studies of graphene and topological insulators.
Dr. Daniel Niesner, University of Erlangen, Germany

25/06/2013
Nanosources, photons and disorder: Nano-optics in complex media.
Prof. Rémi Carminati, Institut Langevin, ESPCI ParisTech, Paris, France

11/07/2013
The Alba light source. Present status and perspectives.
Prof. Salvador Ferrer Fabregas, Synchrotron ALBA, Cerdanyola del Valles, Spain

17/07/2013
Orientation and coupling of adsorbed aromatic molecules by theoretical spectroscopy.
Prof. Guido Fratesi, Universidad degli Studi di Milano-Bicocca, Milano, Italy

19/07/2013
A theoretical perspective of black-holes: past and present.
Dr. Martin Reiris Ithurralde, Max Planck Institute for Gravitational Physics, Golm, Germany

23/07/2013
Nitric oxide as a non-innocent ligand in (bio-)inorganic complexes: charge transfer resolution.
Prof. Ewa Broclawik, Jagiellonian University, Faculty of Chemistry, Krakow, Poland

24/07/2013
The Dielectric Response of Multilayer Graphene Nano-Cones.
Dr. Fredrik Hage, STFC Daresbury Laboratories, Warrington, United Kingdom

07/08/2013
Managing photons and phonons with nanostructures.
Prof. Nikolaos Stefanou, National and Kapodistrian University of Athens, Greece

06/09/2013
Quasiparticle spectra and excitons in organic molecules deposited on graphene and metal surfaces: G0W0-BSE approach.
Dr. Vito Despoja, University of Zagreb, Croatia

10/09/2013
Will Silicene Be the Next Silicon?
Prof. Guy Le Lay, CINaM, Aix-Marseille University, Marseille, France & CNR-ISM, Rome, Italy

16/09/2013
Nanophotonics Enabled by Plasmonic Metamaterials and Nanolasers.
Prof. Shangjr Gwo, National Tsing-Hua University, Taiwan

17/09/2013
A Quantum processor with trapped (Rydberg) ions.
Prof. Markus Hennrich, Institute for Experimental Physics, University of Innsbruck, Austria

20/09/2013
DFT study of strain effects in lanthanum nickelate.
Prof. Bo Hellsing, Chalmers and Göteborg University, Sweden

26/09/2013
Through the quantum world by quantum simulations: from nanotransistors, via multiferroics to graphene and topological insulators.
Dr. Igor Popov, School of Physics, Trinity College Dublin, Ireland

30/09/2013
First-principles inelastic transport using tranSIESTA calculations and user interfaces for the commercial version of the code.
Dr. Mads Engelund, DTU, Copenhagen, Denmark

21/10/2013
Cement under the nanoscope.
Prof. Roland Pellenq, MIT, Massachusetts, USA

28/10/2013
Spin-current generation in metals, semi-, and superconductors.
Dr. Martin Gradhand, University of Bristol, UK

08/11/2013
Linear-scaling approaches to charge- and energy-transfer in (extended) photo-electro-chemical interfaces.
Prof. Gilberto Teobaldi, University of Liverpool, UK

19/11/2013
Conserving approximations for correlated inhomogeneous systems; from molecules to quantum transport.
Dr. Adrian Stan, Détaché à Laboratoire des Solides Irradiés, École Polytechnique, Palaiseau, France

22/11/2013
Electron Acceptor Molecules deposited on epitaxial graphene studied by means of Low temperature scanning tunneling microscopy/spectroscopy
Dr. Manuela Garnica Alonso, IMDEA Nanociencia, Madrid

04/12/2013
X-ray spectroscopy of 3d magnetic impurities on graphene and graphite: from strong to weak interaction.
Dr. Jan Honolka, Institute of Physics, Academy of Sciences of the Czech Republic (ASCR), Prague, Czech Republic

13/12/2013
Soft x-ray spectroscopy for solar energy conversion.
Dr. Ioannis Zegkinoglou, Lawrence Berkeley National Laboratory, California, USA

Workshops 12/13

2012

2013

1st Baskrete Industry Open Days

March 13-14, 2012

ORGANIZERS
Andrés Ayuela (DIPC, Spain)
Jorge S. Dolado (Tecnalia, Spain)

We presented our research in the field of nanoscience and nanotechnology for cementitious materials to local and international cement companies. The speakers provided practical insights to their research and discussion with industry offered trends for better applied research.

CONTRIBUTIONS

Welcome to DIPC (Pedro M Echenique and Ricardo Díez Muiño, DIPC)
The nanoBasque Strategy: a vision of the future (Agencia nanoBasque-SPRI)
The nanoIKER project (Jose M Pitarke, CIC nanoGUNE)
The Baskrete network (Jorge S Dolado, Tecnalia)

Hydration of Clinker
Reactive Force Field Molecular Dynamics to Simulate the Hydration of Calcium Silicate Minerals (Hegoi Manzano, UPV/EHU)
Atomistic simulations of anisotropic etching (Miguel Ángel Gosalvez, DIPC)

Formation and Growth: C-S-H gel & crystalline phases
Monte-Carlo models of cement setting (Raquel González-Teresa, Tecnalia)
DFT simulations of Ettringite (Andrés Ayuela, DIPC)

Nano – Confined Water
Nano-confined water (Silvina Cerveny, CFM)
Challenges and progress in the atomistic simulation of liquid water and wet interfaces (Emilio Artacho, CIC nanoGUNE)

Industrial Experiences
Research & Development at Lafarge (Ellis Gartner, Lafarge)
Rheometry as a tool for inestigating the Microstructure of Cement-based materials (Maurizio Belloto, Bozzetto Group)

Performance & Characterization
29Si NMR spectroscopy on cements: A theoretical study on CSH gel (Pawel Rejmak, DIPC)
Calcium leaching: A computational description (Juan José Gaitero, Tecnalia)

Non-Portland Cements
The C-A-S-H gel of the Alkali Activated Cements (Jorge S. Dolado, Tecnalia)

Organic - Inorganic Interactions
A first atomistic attempt... (Hegoi Manzano, UPV/EHU)
The soft hardening of cements (Jorge S. Dolado, Tecnalia)

Nano-Additions and Nano - Reinforcements
Can cementitious nanotubes exist? (Andrés Ayuela, DIPC)
Self-healing cement-based materials (Edurne Erkizia, Tecnalia)

Andreev Bound States and More

July 4-6, 2012

ORGANIZERS
Sebastian Bergeret (Centro de Física de Materiales CSIC-UPV/EHU, Spain)
Cristian Urbina (CEA, Saclay, France)

This workshop brought together a group of leading scientists actively working on the detection and modeling of Andreev Bound Sates in superconducting nanostructures.

CONTRIBUTIONS

Caglar Girit (CEA, Saclay, France)
Microwave spectroscopy of Andreev states in atomic contacts

Yuli Nazarov (University of Delft, Netherlands)
Singlet-Triplet manipulation of Andreev states in break junctions

Landry Bretheau (CEA, Saclay, France)
Modeling of spectroscopy of an atomic SQUID using a Josephson on-chip detector

Vitaly Shumeiko (Chalmers, Göteborg, Sweden)
Relaxation processes in Andreev levels system

Manuel Houzet (CEA, Grenoble, France)
Spin-boson description of the Andreev levels microwave spectroscopy experiments

Marcelo Goffman (CEA, Saclay, France)
Andreev Bound States and Kondo effect in carbon nanotubes

Alfredo Levy Yeyati (Universidad Autonoma de Madrid, Spain)
Interaction effects in Andreev and Majorana bound states in quantum dots

Guillermo Romero (UPV/EHU, Bilbao, Spain)
Circuit Quantum Electrodynamics with a Superconducting Quantum Point Contact

Andrew Doherty (University of Sydney, Australia)
A master equation approach to P(E) theory for the dynamical Coulomb blockade

Juan Carlos Cuevas (Universidad Autonoma de Madrid, Spain)
Microwave-assisted supercurrents and ac response of superconducting nanostructures

Fabio Pistolesi (University of Bordeaux, France)
Detection of ultrafast mechanical oscillations by exploiting Andreev bound states in superconducting junctions

Alvise Verso (DIPC, Spain)
Josephson current through a spin-filter

Philippe Joyez (CEA, Saclay, France)
Andreev Bound States and Kondo effect in carbon nanotubes

Hugues Pothier (CEA, Saclay, France)
Modeling of spectroscopy of an atomic SQUID using a Josephson on-chip detector

NFO12
The 12th International Conference on Near-field Optics, Nanophotonics and related techniques

September 3-7, 2012

ORGANIZERS
Javier Aizpurua (DIPC and CSIC-UPV/EHU, Spain)
Rainer Hillenbrand (CIC nanoGUNE and Ikerbasque, Spain)

We celebrated the 20th anniversary of the international conference of Near-field Optics, Nanophotonics and Related Techniques (NFO) since its first edition in 1992. NFO has been among the first conferences addressing optics on the nanometer scale, triggered by the fascinating prospects of near-field techniques for pushing the resolution of optical microscopy towards the molecular level. Twenty years later, a variety of novel fields that involve nanooptics and photonics have been developed, including plasmonics, metamaterials, quantum information, biosensing and ultrafast dynamics. NFO12 covered all these fields, providing an international platform to present and discuss the latest advancements.

CONTRIBUTIONS

Martin Aeschlimann (University of Kaiserlauten, Germany)
Ultrafast optical control at the nanoscale

Dimitry N Basov (UC, San Diego, USA)
Dirac plasmons in graphene: spectroscopy and imaging

Philip E Batson (Rutgers, The State University of New Jersey, USA)
Plasmonic Forces Induced by Swift Electrons in Small Particles

Jeremy Baumberg (University of Cambridge, United Kingdom)
Quantum Plasmonics in gap plasmons with precise sub-nm control

Oliver Benson (Humboldt University, Berlin, Germany)
Fundamental Photonic Hybrid Systems Based on Defect Centers in Diamond

Richard Berndt (University of Kiel, Germany)
Coupled plasmons at the transition from tunnelling to contact

Alexandre Bouhelier (Université de Bourgogne, Dijon, France)
X(2) processes in electrically contacted optical gap antennas: second harmonic generation and optical rectification

Yannick De Wilde (CNRS, ESPCI, Paris, France)
NSOM applications to plasmonics at infrared wavelength

Enzo Di Fabrizio (Istituto Italiano di Tecnologia, Genoa, Italy)
Nanostructures and their use in nano optics

ZhenChao Dong (University of Science and Technology of China, Hefei, China)
Plasmon mediated single molecular optoelectronics

Jens Dorfmüller (University of Stuttgart, Germany)
Real-Space Imaging of Optical Nanoantennas by apertureless SNOM

Wolfgang Fritzsche (IPTH Jena, Germany)
Biosensing at the single particle level

Javier García De Abajo (Institute of Optics, Madrid, Spain)
Graphene plasmonics: An atomically thin look into NFO

Francisco García-Vidal (Universidad Autónoma de Madrid, Spain)
Localized spoof surface plasmons in textured particles

Harald Giessen (Universität Stuttgart, Germany)
Complex plasmonic nanostructures: moving towards applications

Haewook Han (Postech, South Korea)
Quantitative Spectroscopic Terahertz Near-Field Microscopes

Achim Hartschuh (LMU Munich, Germany)
New directions in tip-enhanced near-field optical microscopy

Christiane Hoeppener (University of Münster, Germany)
Single Sphere and Self-similar Colloidal Nanoparticle Antennas for Membrane Protein Imaging

Mikael Käll (Chalmers University, Sweden)
Nanoplasmonic biosensing – promises and problem

Femius Koenderink Amolf (Netherlands)
Near-field measurement and manipulation of antenna-enhanced spontaneous emission

Frank Koppens (ICFO, Barcelona, Spain)
Graphene plasmonics

Joachim Krenn (University of Graz, Austria)
Tuning plasmon modes for biosensing

Kristján Leosson (University of Iceland)
New fabrication approaches in low-loss plasmonics and controlled self-assembly of metal nanostructures for biosensing

Mikhail Lukin (Harvard University, Massachusetts, USA)
Nanophotonics meets quantum optics

Adnen Mlayah Cemes (Toulouse, France)
Acousto-Plasmonics based sensing

Hrvoje Petek (University of Pittsburgh, Pennsylvania, USA)
Ultrafast plasmonics: Imaging light with electrons on the femto-nano scale

Albert Polman Amolf, Netherlands)
Angle-resolved cathodoluminiscence imaging Spectroscopy:
deep subwavelength imaging of the modal dispersion of light

Anne Marie Pucci (Universität Heidelberg, Germany)
Surface enhanced infrared spectroscopy

Romain Quidant (ICFO, Barcelona, Spain)
Towards an integrated plasmonic platform for early cancer diagnosis

Mark Stockman (Georgia State University, Atlanta, USA)
Spasing and Amplification in Plasmonic Nanosystems

Yung Doug Suh (Korea Research Institute Of Chemical Technology, Republic of Korea)
Nano-gap Enhanced Raman Scattering (NERS) controlled by DNA

Prabhat Verma (Osaka University, Japan)
High-resolution optical imaging through plasmonics and beyond plasmonics

Hong Wei (Chinese Academy of Sciences, Beijing, China)
Controlling Surface Plasmon Modulations in Siver Nanowire Waveguides

Kumar Wickramasinghe (UC Irvine, California, USA)
Raman Probe Force Microscopy — a New Method to Detect the Raman Effect

Jörg Wrachtrup (Universität Stuttgart, Germany)
Near field imaging with single atomic emitters

Joel Yang (Institute of Materials Research and Engineering, Singapore)
Driving Resonances In Plasmonic Nanoantennas By Electrons and Photons

Superconducting Nanohybrids 2012

September 3-7, 2012

ORGANIZERS
Sebastian Bergeret (Material Physics Center, CFM, Spain)
Alexander Golubov (University of Twente, Netherlands)
Andrei Zaikin (Karlsruhe Institute of Technology, Germany)

This workshop brought together leading scientists actively working in different sub-fields of mesoscopic superconductivity in order to discuss recent advances and overview the present status of the field, to visualize further research prospects and to promote new collaborations. The program will included talks by leading experts, both theorists and experimentalists, in topics such as: Unconventional pairing in superconductor-ferromagnet proximity structures, Proximity and Josephson effects in carbon nanotubes, graphene and topological insulator, Superconducting quantum dots, Quantum phase slips in superconducting nanowires and nanorings, Crossed Andreev reflection in NS and FS structures, Novel superconductors ,Spintronics and superconductivity, Superconductivity and thermoeffects

CONTRIBUTIONS

Teunis Martien Klapwijk (TU Delft, Netherlands)
The evolution of superconducting hybrids

Leonid S Kuzmin (Chalmers University of Technology, Sweden)
2D Arrays of Cold-Electron Bolometers for High- Performance Cosmology Experiments

Pertti Hakonen (Aalto University, Helsinki, Finland)
Hybrid Circuit Cavity Quantum Elctrodynamics with a Micromechanical Resonator

Mikhail S. Kalenkov (Lebedev Physical Institute, Russian Academy of Sciences, Moscow, Russia)
Giant thermoeffect in superconductors with magnetic impurities

Matthias Eschrig (Royal Holloway University of London, United Kingdom)
Giant Nonlocal Thermoelectric Effects in Three-terminal Superconducting Devices

Francesco Giazotto (Scuola Normale Superiore-CNR, Pisa, Italy)
Realizing heat interferometry through the Josephson effect

Pauli Virtanen (University of Würzburg, Germany)
Absorption of heat into a superconductor —normal metal— superconductor junction from the electromagnetic environment

Clemens Winkelmann (Neel Institute, France)
Electronic refrigeration and thermal couplings in superconducting hybrid devices

Konstantin Yu Arutyunov (University of Jyväskylä, Finland)
Quantum phase slip junction

Oleg Astafiev (NEC Research Laboratories, Tsukuba, Japan)
Coherent quantum phase slips in superconducting nano-wires

Frank Hekking (University Joseph Fourier, Grenoble, France)
Quantum phase-slips in Josephson junction rings

Carmine Attanasio (University of Salerno, Italy)
Quantum phase slips in superconducting Nb nanowire networks deposited on self-assembled Si templates

Evgeni Il'ichev (Jena, Germany)
Dressed state amplification by a superconducting qubit

Julia Meyer (CEA-Grenoble,France)
Andreev current induced by ferromagnetic resonance

Andrei Semenov (Lebedev Physics Institute, Moscow, Russia)
Subgap electron transport in superconducting hybrids and Cooper pairs dephasing by electron-electron interactions

Venkat Chandrasekhar (Northwestern University, USA)
Nonlocal correlations in a proximity-coupled normal metal

Tero Heikkilä (Aalto University, Finland)
Manifestly non-Gaussian temperature fluctuations in superconductor-normal metal-superconductor structures

François Lefloch (CEA-Grenoble, France)
Transport properties of diffusive three terminal hybrid superconducting S-N-S-N-S nanostructures

Jan Aarts (Leiden University, Netherlands)
Aarts Long-ranged supercurrents in ferromagnetic CrO_2

Victor Petrashov (Royal Holloway Un.of London, United Kingdom)
Superconducting phase coherent electron transport in nano-engineered ferromagnetic vortices

Shiro Kawabata (National Institute of Advanced Industrial Science and Technology, Japan)
A robust odd-frequency paring in ferromagnet/superconductor junctions

Norman Birge (Michigan State University, USA)
Spin-triplet supercurrent in ferromagnetic Josephson junctions

Mark Blamire (Cambridge University, United Kingdom)
Spin currents in superconductors

Alvise Verso (Donostia International Physics Center, Spain)
Spin-polarized Josephson and quasiparticle currents in superconducting spin-filter tunnel junctions

Alexander Brinkman (University of Twente, Netherlands)
Josephson supercurrent through a topological insulator surface state

Manuel Houzet (CEA- Grenoble, France)
Topological Josephson junctions out of equilibrium

Yasuhiro Asano (Hokkaido University, Japan)
Majorana Fermions and Odd-frequency Cooper Pairs

Alexander Buzdin (University of Bordeaux, France)
Vanishing Meissner effect as a hallmark of in-plane FFLO instability in superconductor-ferromagnet layered Systems

Avradeep Pal (University of Cambridge, United Kingdom)
Spin filter tunnel junctions with superconducting electrodes Mohammad Alidoust:
Unusual current-phase relation and magnetic interference pattern in non-aligned Josephson junctions

J Samuel Jiang (Argonne, USA)
Unconventional proximity effect in ferromagnet/superconductor heterostructures with controlled magnetic non- collinearity

Jason Robinson (University of Cambridge, United Kingdom)
Supercurrent enhancement in Bloch-like domain walls

Lenar Tagirov (Kazan University, Russia)
Experimental Observation of the Triplet Spin-Valve Effect in a Superconductor-Ferromagnet Heterostructure

Anna Suszka (nanoGune, San Sebastian, Spain)
Complex response of superconductivity to inhomogeneous magnetization states in epitaxial Nb/[DyFe2/YFe2]23 multilayer

Yakov Fominov (Landau Institute, Russia)
Odd-frequency-diamagnetic vs. odd-frequency- paramagnetic superconductivity

Valerii Vinokur (Argonne National Laboratory, USA)
Magnetic field induced superconductivity in nanostructures

Mario Cuoco (CNR-SPIN, Italy)
Odd-Frequency Triplet Pairing in Mixed-Parity Superconductors and in the presence of Rashba interaction

Audrey Cottet (CNRS Paris, France)
Inducing triplet superconducting correlations in a normal metal wire

Detlef Beckmann (Karlsruhe Institute of Technology)
Long-range spin transport in superconductors

Jukka Pekola (Aalto University, Finland)
Statistics Of Dissipation In Superconducting Tunneling

Valery Ryazanov (Institute of Solid State Physics, Russia)
Double proximity effect in hybrid planar Superconductor-(Normal metal/Ferromagnet)-Superconductor structures

Charis Quay Huei Li (Université Paris-Sud, France)
Spin Imbalance and Spin-Charge Separation in a Mesoscopic Superconductor

Edward Goldobin (Tübingen University, Germany)
Josephson junctions with magnetic field tunable current-phase relation

JCNS and DIPC Joint Workshop: Trends and Prespectives in Neutron Scattering for Soft Matter and Biophysics

October 8-11, 2012

ORGANIZERS
Dieter Richter (Jülich Centre for Neutron Science, Germany)
Juan Colmenero (Centro de Física de Materiales CSIC-UPV/EHU and DIPC, San Sebastián, Spain)

Neutron scattering has proven to be a key method to get deep insight into soft matter physics, biophysics and soft matter molecular structures . A comprehensive set of techniques is used to reveal the structure and dynamics of polymers, colloids, polymer interfaces, polymer composites and glasses as well as biomolecules, biocompatible and bio - mimetic structures . The aim of the international workshop jointly organized by the Jülich Centre for Neutron Science and the Donostia International Physics Center is to discuss the current status and the future trends and challenges of neutron scattering in this field The workshop will bring experts together to address the following topics: Advanced Instrumentation for Soft Matter Research, Physics of Life, Kinetic Processes, Soft Materials for Energy Devices, Sustainable Polymers, Functional Materials, Synergies between Neutrons and Simulation, Nanostructured Systems

CONTRIBUTIONS

Luigi Paduano (University of Naples "Federico II", Italy)
Nanodevices for antineoplastic diagnosis or therapy

Michael Gradzielski (Technische Universität Berlin, Germany)
Structure and dynamics of polyelectrolyte/surfactant complexes probed by SANS and NSE and their relation to the rheological properties

Mitsuhiro Shibayama (The University of Tokyo, Chiba, Japan)
Structure and gelation dynamics of tetra-PEG ion gels

Volker Urban (Oak Ridge National Laboratory, Tennessee, USA)
Neutron scattering for energy and the environment – light harvesting biofuels

Satoshi Koizumi (Ibaraki University, Hitachi, Japan)
In-situ observation of operating polymer electrolyte fuel cells (PEFC) by neutron small angle scattering – contrast variation by using deuterium gas

Regine von Klitzing (Technische Universität Berlin, Germany)
Stimuli sensitive polymer coatings with different film architectures

Stephan Förster (Universität Bayreuth, Germany)
Structure of soft lyotropic crystals and quasicrystals

Matthias Ballauff (Helmholtz Zentrum Berlin, Germany)
Small-angle neutron scattering – recent results on colloids and future trends

Sanat Kumar (Columbia University, New York, USA)
Modeling polymer nanocomposite structure and dynamics

Alessandro Paciaroni (University of Perugia, Italy)
Elastic and quasielastic neutron scattering investigation of biomolecules in glassy environments

Ralf Biehl (Forschungszentrum Jülich, Germany)
Proteins in solution: determination of domain structure and dynamics

Maikel Rheinstädter (McMaster University, Hamilton, Canada)
Frontiers in membrane biophysics

Victoria Garcia Sakai (ISIS, Didcot, United Kingdom)
Views from a soft matter neutron instrument scientist

Bernhard Frick (Institut Laue Langevin, Grenoble, France)
New developments in neutron backscattering with applications in soft matter and perspectives for studies of slow dynamics

Juan Colmenero (Centro de Física de Materiales CSIC-UPV/EHU and DIPC, San Sebastián, Spain)
Chain dynamics in un-entangled polymer blends with dynamic asymmetry.
A generalized Rouse incoherent scattering function based on the GLE formalism

Isabelle Grillo (Institut Laue Langevin, Grenoble, France)
Recent applications of time resolved SANS combined with a stopped-flow equipment

Toshiji Kanaya (Kyoto University, Japan)
Flow-induced polymer crystallization – effects of molecular weight and shish-kebab formation

Surface Dynamics:
Beyond the Born-Oppenheimer Static Surface Approximation

October 24-26, 2012 | Universidad de Zaragoza, Spain

ORGANIZERS

Cristina Díaz (Universidad Autónoma de Madrid, Spain)
Manuel Alcamí (Universidad Autónoma de Madrid, Spain)
Sergio Díaz-Tendero (Universidad Autónoma de Madrid, Spain)
Maite Alducin (CSIC-UPV Materials Physics Center and DIPC, San Sebastián, Spain)
Roar A. Olsen (SINTEF Materials and Chemistry, Oslo, Norway)

To present, most of the study performed on molecule/surface interactions have taken advantage of the Born-Oppenheimer static surface (BOSS) approximation. To unravel the role played by non-adiabatic effects on these systems represents a new challenge for surface science physicists. Evidence of non-adiabatic effects has been found, for example, for metal with low work functions through chemicurrents measurements. But, the main question to be answered now is relative to the role that electron hole pair excitations could play in reactive and non-reactive scattering of molecules, both openshell and close-shell ones, with metal surfaces, and to the role played by phonon excitations.

The scope of this workshop has been to serve as meeting point for theoretical and experimental scientists working on the field, which allows them to identify problems of interest for experimentalist, to identify bottlenecks on actual theoretical methods, and to exchange new ideas that could be used to overcome some of the actual shortcomings. This objective has been fully fulfilled, thanks to the good balance between theoretical and experimental talks at the workshop. The experimentalists have pointed out the need to go beyond the Born-Oppenheimer static surface (BOSS) approximation in order to properly describe, for example, phenomena relative to femtochemistry. The workshop has also allowed to establish the state-of-the-art of the development on nonadiabatic dynamical methods.

CONTRIBUTIONS

Rainer Beck (Ecole Polytechnicque fédérale de Lausanne, Switzerland)
State-resolved gas/surface reactivity measurements: evidence for mode- and bond selective chemisorption of methane on Ni and Pt

Eckart Hasselbrink (Universität Duisburg-Essen, Germany)
Non-Adiabaticity in Surface Chemical Reactions Studied Using Thin Metal Film Heterostructures

Alberto Pablo Sánchez Muzas (Universidad Autónoma de Madrid, Spain)
Vibrational deexcitation and rotational excitation of H_2 and D_2 scattered from Cu(111): adiabatic versus non-adiabatic dynamics

Paul Tiwald (Vienna University of Technology, Austria)
Charge exchange between a proton and a lithium fluoride surface: an embedded cluster approach

Fernando Martin (Universidad Autónoma de Madrid, Spain)
Commensurate solid-solid phase transitions in self-assembled monolayers of alkylthiolates lying on metal surfaces

Alec Wodtke (Max Planck Institute for Boiphysical Chemistry, Germany)
Surface Dynamics: Beyond the Born-Oppenheimer Static Surface Approximation

Daniel Auerbach (University of California, USA)
on-adiabatic electronic effects in energy transfer at metal surfaces: do we need to go beyond electronic friction models?

Iñaki Juaristi (UPV/EHU, Spain)
Role of energy loss channels in the reactive and non-reactive dynamics of molecules and atoms on metal surfaces

Peter Kratzer (Univerisity Duisburg-Essen, Germany)
Energy dissipation at surfaces by anharmonic vibrational coupling and electron-hole pair excitation

Pascal Larregaray (ISM, UMR5255, CNRS/U.Bordeaux1, France)
Dynamical reaction pathways in Eley-Rideal recombination of Nitrogen from W(100)

Francesco Nattino (Leiden Institute of Chemistry (LIC), Leiden University, Netherlands)
Ab-Initio Molecular Dynamics study of CHD_3 dissociation on Pt(111): the role of the v1-normal mode pre-excitation

Remi Petuya (ISM, UMR5255, CNRS/U.Bordeaux1, France)
Theoretical analysis of the dynamics of N_2 scattering on W(100) surface

Maitreyi Robledo Relaño (Universidad Autónoma de Madrid, Spain)
Charge transfer in molecules and ultrathin insulating films deposited on metal surfaces

Phillip Thomas (Leiden University, Netherlands)
Sum-of-Products Representation of Potential Energy Surfaces using the Chebyshev n-mode Approach: Application to 6D Gas-Surface Reactive Scattering Problems

Martin Wolf (Fritz Haber Institute, Berlin, Germany)
From surface femtochemistry to ultrafast phase transitions in CDW systems

Peter Saalfrank (Institut für Chemie, Universität Postdam, Postdam-Golm, Germany)
Vibration-phonon and vibration-electron hole pair coupling at surfaces

Maria Blanco-Rey (DIPC, Spain)
Vibrational excitation of hydrogen atoms in palladium by ballistic electrons

Rachel Crespo-Otero (Max-Planck-Institut für Kohlenforschung, Germany)
Photochemistry of N-Methylformamide: Matrix Isolation and Nonadiabatics Dynamics

Jean-Pierre Gauyacq (Université de Paris-Sud, France)
Magnetic (spin) transitions in adsorbates at surfaces induced by tunnelling electrons

Thomas Frederiksen (DIPC, Spain)
Theory and simulation of vibrational spectroscopy and adsorbate dynamics with inelastic tunneling electrons

Thorsten Kluener (University of Oldenburg, Germany)
Ab-initio surface photochemistry

Myrta Grüning (University of Coimbra, Portugal)
Ab-initio many-body perturbation-theory: overview and perspectives

Geert-Jan Kroes (Leiden Institue of Chemistry, Leiden University, Netherlands)
Quantum and Ab Initio Molecular Dynamics calculations on scattering of H atoms and H_2 molecules from metal surfaces

Daniel Farías (Universidad Autónoma de Madrid, Spain)
Molecular beam studies of the dissociation of H_2 and O_2 on metal surfaces

Mark Wijzenbroek (Leiden Institute of Chemistry, Leiden University, Netherlands)
Static surface temperature effects on the dissociation of H_2 and D_2 on Cu(111)

Joerg Meyer (Technische Universität München, Germany)
Better than the BOSS: Watching phonons cool down during oxygen dissociation on Pd(100)

Controlled Atomic Dynamics on Solid Surfaces: Atom and Molecular Manipulation

May 13-16, 2013

ORGANIZERS
Thomas Frederiksen (DIPC, San Sebastián, Spain)
Nicolás Lorente (CIN2, Barcelona, Spain)
Magnus Paulsson (Linnaeus University, Sweden)

The objective of this workshop was to provide a thorough picture of the existing theoretical techniques and how they are contributing to the understanding and quantitative prediction of controlled manipulations. Equivalently, the workshop aims at exposing present experimental developments and challenges that need to be addressed by new theoretical developments. The meeting will steer discussions and collaborations much needed to add momentum to a developing field. This workshop can be of landmark importance since no equivalent workshop or conference has been organized with the aim of making "controlled manipulations" a full-fledged research field.

This workshop was dedicated to Prof. Hiromu Ueba and to all of his contributions to this field.

CONTRIBUTIONS

Maite Alducin (CFM-CSIC, San Sebastián, Spain)
Does N_2 adsorption increase on strained Fe monolayers?

Richard Berndt (Kiel University, Germany)
Manipulation of the spin and charge states of adsorbed molecules

María Blanco-Rey (DIPC, San Sebastián, Spain)
Subsurface Hydrogen and Deuterium Manipulation by Ballistic Electrons

Marie-Laure Bocquet (ENS Lyon, France)
Understanding Inelastic Electron Spectroscopy of single adsorbates on metal surfaces: start «small», finish «big»

Mads Brandbyge (DTU Nanotech, Denmark)
Electron-Phonon coupling and molecular dynamics in the presence of current

Eugene Chulkov (CSIC-UPV/EHU, Spain)
Relativistic effects in surface electronic structure of solids: Bychkov-Rashba systems and topological insulators

Karl-Heinz Ernst (EMPA, Switzerland)
Chirality in molecular recognition and dynamics at surfaces

Aran Garcia-Lekue (DIPC, San Sebastián, Spain)
Azobenzene-Based Single-Molecule Junctions:Charge Transport Mechanism and IETS Fingerprints

Michael Galperin (UC San Diego, USA)
Molecular junctions: A nonequilibrium atomic limit

Jean-Pierre Gauyacq (CNRS Paris-Sud, France)
Excitation of magnetic adsorbates by tunnelling electrons: atoms and chains

Axel Gross (Ulm University, Germany)
Molecule-surface interactions at complex metal-gas and metal-liquid interfaces studied by ab initio molecular dynamics simulations

Werner Hofer (Liverpool University, UK)
Theory of scanning tunneling microsopy: studying dynamic processes

Maki Kawai (RIKEN, Tokyo, Japan)
Local Symmetry Rules Spin Ground State: FePc on Au(111)

Tadahiro Komeda (Tohoku University, Japan)
Manipulation of Spin in Double Decker Phthalocyanine Molecule

Rolf Möller (Duisburg-Essen University, Germany)
Revealing molecular dynamics through scanning noise microscopy and spectroscopy

Karina Morgenstern (Ruhr-Universität Bochum, Germany)
Inelastic spectroscopy with sub-atomic resolution

Hiroshi Okuyama (Kyoto University, Japan)
Controlled switching molecule-electrode interfaces

Richard Palmer (Birmingham University, UK)
Atomic manipulation by electron injection

Jose-Ignacio Pascual (CIC nanoGUNE, San Sebastián, Spain)
Spin, Forces and Photons in Molecular Tunneling Junctions

Bo Persson (Forschungszentrum Jülich, Germany)
Charging and Bond formation of Adsorbates on Ultrathin, Insulating Films Supported by a Metal Substrate

Mats Persson (Liverpool University, UK)
Tribology at the atomistic level

Hrvoje Petek (Pittsburgh University, USA)
A multi-state single-molecule switch actuated by rotation of an encapsulated cluster within a fullerene cage

Roberto Robles (CIN2, Spain)
Site- and orbital-dependent charge and spin manipulation in supported transition metal phthalocyanines

Ruslan Temirov (Forschungszentrum Jülich, Germany)
Imaging and control of large organic molecules within a scanning probe microscopy junction

Sergei Tikhodeev (GPI Moscow, Russia)
Mechanisms of rotation of a single acetylene molecule on Cu(001) by tunneling electrons in STM

Tchavdar Todorov (Queens University Belfast, UK)
Interatomic forces under current

Hiromu Ueba (Toyama University, Japan)
Vibrationally mediated single molecule reactions in real space and in real time

Martin Wolf (Fritz-Haber MPG, Berlin, Germany)
Probing the transient electronic structure in surface femtochemistry

2nd Baskrete Industry Open Days

May 28-29, 2013

ORGANIZERS
Andrés Ayuela (DIPC, Spain)
Jorge S. Dolado (Tecnalia, Spain)

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), the 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.

The Baskrete Open Days target to industrials but it will be relevant to anyone (in academia, national research institutes or industry) with experience/expertise in cementitious materials and anyone interested in the latest achievements and about the short and long term prospects in this promising field.

Baskrete acknowledges the funding received from NANO-IKER project (IE11-304), within the Etortek program of the Department of Industry, Innovation Trade and Tourism of the Basque Government.

CONTRIBUTIONS

P.M. Echenique and R.Díez Muiño (DIPC)
Welcome to DIPC

A. Martinez Muro (nanoBasque)
EHS Advance, safety nanotechnologies for companies

J. Campas (Euskampus)
Euskampus: community of Knowledge poles

J.S. Dolado (Tecnalia)
The Baskrete initiative

S. Shah (Northwestern University, USA)
Nanomodification of cementitious materials with nanaoparticles

H. Manzano (UPV/EHU)
Hydration of clinker phases using molecular simulations

A. Ayuela (DIPC)
Structure, atomistic simulations and phase transitions of stoichiometric yeelemite

J.S. Dolado (Tecnalia)
Early growth of C-S-H gel

J.J. Gaitero (Tecnalia)
Aging and durability of ternary cements containing fly ash and activated paper sludge

M. Belloto (Bozzetto Group)
Superfluid pumpable concrete:
the role of superplasticizers on performances, robustness and chesiveness

P. Rejmak (DIPC)
29Si chemical shift anisotropies in hydrated calcium silicates: a computational study

H. Manzano (UPV/EHU)
Sheer deformations in the C-S-H gel: understanding the moleclar mechanism of creep

J.S. Dolado (Tecnalia)
Multi-scale modeling of cement-based materials: structure performance linkage

A. Ayuela (DIPC)
Do cementitious nanotubes exist?

30th Brandt Ritchie Workshop (BRW)

October 1-4, 2013

ORGANIZERS
Andres Arnau (CFM CSIC-UPV/EHU and DIPC, Spain)
Joseba Iñaki Juaristi (CFM CSIC-UPV/EHU and DIPC, Spain)
Pedro Miguel Echenique (DIPC and CFM CSIC-UPV/EHU, Spain)

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John R. Sabin (University of Florida, USA)
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Helmut Winter (Humboldt University, Germany)
Vladimir Esaulov (ISMO, France)
Jorge Valdés (USM, Valparaíso, Chile)
Fernando Flores (UAM, Spain)
Yasunori Yamazaki (RIKEN, Japan)

The topics within BRW cover various fields of condensed matter physics or material science, In particular, the following subjects were addressed: Particle-solid interactions with special attention to charge exchange, energy loss and related phenomena; collective excitations in low-dimensional systems; induced excitation of surface and bulk plasmon states; dynamic charge states in ion-solid interactions; electron dynamics in nanostructures; photonic and transport properties of materials; radiation interaction with organic and inorganic nano-materials; related processes at surfaces, interfaces and nanostructures. Following the spirit of previous Brandt Ritchie Workshops, participants presented recent results of their research activity.

This edition paid homage to Rufus Ritchie, an outstanding physicist, who has realized seminal contributions to the fields of atomic physics and interaction of atoms with matter. Prof. Rufus Ritchie was given an honorary degree from the University of the Basque Country.

The BRW workshop took place at Donostia International Physics Center (Donostia-San Sebastián).

CONTRIBUTIONS

Peter Bauer (JKU Linz, Austria)
Electronic stopping of slow light ions in metals and insulators

Aitor Bergara (UPV/EHU, Spain)
Emergence of new low-energy plasmons under pressure

María S. Gravielle (Instituto De Astronomía y Física del Espacio (IAFE), Argentina)
Grazing incidence fast atom diffraction from metal surfaces

Natalia E. Koval (Centro De Física De Materiales and Consejo Superior de Investigaciones Científicas, Spain)
Energy loss and charge transfer processes during photoemission from metal clusters and adsorbates

Sir John B. Pendry (Imperial College London, United Kingdom)
Challenges in Surface Plasmonics

Fernando Flores (Universidad Autónoma de Madrid, Spain)
Inelastic tunneling spectroscopy for magnetic atoms and the Kondo resonance

Archie Howie (University of Cambridge, United Kingdom)
Thermal Fluctuations and Decoherence in Electron Microscopy

Christoph Lemell (Vienna University of Technology, Austria)
Classical simulations for surface-streaking experiments

Karoly Tokesi (MTA Atomki, Hungary)
Can the ions be guided with MeV/amu energies? The case of 1 MeV proton microbeam

Vito Despoja (University of Zagreb, Croatia)
Electron loss and photoemission spectra in pristine and doped graphene

Jorge Esteban Miraglia (Instituto de Astronomía y Física del Espacio, Argentina)
Electron impact multiple ionization

Raúl Antonio BARAGIOLA (University of Virginia, USA)
Electron emission by rare gas ions on Cs coated Al surfaces

Julio Ferrón (Intec Conicet Unl, Argentina)
Unoccupied band states and ion induced electron emission

Juana Gervasoni (Cnea-Conicet, Argentina)
Plasmon excitations in single-walled carbon nanotubes by impact of charged particles

María Luz Martiarena (Conicet, Argentina)
Li+ neutralization on nanostructures of Au: size effects on the charge exchange process

Nerea Zabala (UPV/EHU, Spain)
Electromagnetic interaction between relativistic electrons and bounded targets

Amand Lucas (University of Namur, Belgium)
Giant phonon tsunami caused by energetic ions skipping on a polar surface

Andrés Ayuela (Donostia International Physics Center, Spain)
Computational 29Si NMR in Hydrated Portland Cement

Richard A. Wilhelm (Helmholtz-Zentrum Dresden – Rossendorf,
Institute of Ion Beam Physics and Materials Research, Germany)
Interaction of Slow Highly Charged Ions with Free-Standing 1nm Thick Carbon Nano-membranes

Maia G. Vergnori (Donostia International Physics Center, Spain)
Exchange interaction and its tuning in magnetic binary chalcogenides

Aran García-Lekue (Donostia International Physics Center, Spain)
Intermolecular H-Bonding for Porphyrin Molecules on Surfaces

María Blanco Rey (Donostia International Physics Center, Spain)
Efficient Eley-Rideal reactions with large projectiles made possible:
N2 formation by pick-up of N-adsorbates off Ag(111)

John R. Sabin (University of Florida, USA)
Coupled Cluster Calculation of Atomic Mean Excitation Energies

Salvador Cruz-Jimenez (Universidad Autónoma Metropolitana, Mexico)
Study of Many-electron Atom Confinement by Padded Open and Closed Boundaries

Remigio Cabrera-Trujillo (Instituto de Ciencias Físicas, Unam, Mexico)
Universal scaling behavior for the electronic stopping cross section of protons on atomic and molecular targets

Moni Behar (Universidade Federal Do Rio Grande Do Sul, Brazil
Coulomb heating behavior of fast light diclusters through the Si<110> direction:
influence of the mean charge state

Edith Goldberg (Intec Unl Conicet, Argentina)
How do surface energy gaps and image states affect the neutralization of Li+ in the
scattering by metal surfaces?

Laura Isabel Fernández (Donostia International Physics Center, Spain)
Co nanodot arrays grown on a ferromagnetic GdAu2 template:
substrate/nanodot antiferromagnetic exchange coupling

Vyacheslav Silkin (Donostia International Physics Center, Spain)
Acoustic plasmons in extrinsic free-standing graphene

Rosa Monreal (Universidad Autónoma de Madrid, Spain)
Quantum Plasmonics?

Helmut Winter (Humboldt University, Germany)
Recent progress in Fast Atom Diffraction

Rubén Esteban Llorente (Donostia International Physics Center, Spain)
Effect of quantum tunneling in plasmonics: theory and experiments

Andreas Heidenrich (UPV/EHU, Spain)
Coulomb explosion of doped helium clusters

Eduardo C. Montenegro (Ufrj, Rio de Janeiro, Brazil)
Electron loss and energy loss

Jaume Navarro (Department of Logic and Philosophy of Science (UPV/EHU) and Ikerbasque, Spain)
Niels Bohr in Manchester. A hundred years of the quantum atom

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 with more than seventy students who have obtained their Master's degree. Almost 50% of our graduates are international students coming from four different 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.

4th Laboratory Course on Dielectric Spectroscopy

May 20-24, 2013

TEACHERS
Prof. A. Alegría, Dr. S. Arrese-Igor, Dr. D. Cangialosi, Dr. S. Cerveny, and Dr. G.A. Schwartz

The Polymer and Soft Matter Group (PSMG) at Materials Physics Center (CSIC-UPV/EHU) San Sebastián, Spain, organized a laboratory course on broad-band dielectric spectroscopy. The course was open to graduate students and researchers in Physics, Chemistry, Materials Science or Biology and the aim was to introduce participants into the dielectric relaxation experimental techniques and its applications in soft-condensed matter research.

The laboratory course consisted of lectures and experimental sessions. Each lecture included an introduction to polarization theory, dielectric materials and instrumentation. Selected experiments on soft-matter and polymers were conducted and analyzed by the participants. Furthermore, there were two invited tutorials on specific topics involving intensively dielectric relaxation experiments.

LABORATORY SESSIONS

Fundamentals of electrostatics and dielectric materials (S. Cerveny)

Polarization and dielectric permittivity (A. Alegría)

Dielectric relaxation (D. Cangialosi)

Phenomenological models of dielectric relaxation (G.A. Schwartz)

Experimental methods (S. Arrese-Igor)
Laboratory session 1. Introduction
Laboratory session 2. Preparing a first experiment.

Tutorial on: Broadband Dielectric Spectroscopy as a Powerful Tool for Investigating Molecular Dynamics and Proton Reaction Kinetics Of Condensed Matter

Systems at Ambient and Elevated Pressure" by Prof. M. Paluch Institute of Physics, University of Silesia, Poland

Sample preparation procedures (S. Cerveny)
Introduction to data analysis (D. Cangialosi)
Laboratory session 3. Preparing a second experiment

Analysis of experimental data 1
Analysis of experimental data 2
Laboratory session 4. Preparing a third experiment
Analysis of experimental data 3

Analysis of experimental data 4
Summary on data analysis and interpretation (A. Alegría)

http://dipc.ehu.es

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