# dipc2014

Donostia International Physics Center

## THE LYCURGUS CUP

The Lycurgus Cup demonstrates a short-lived technology developed in the fourth century AD by Roman glassworkers. It is the only known complete example of dichroic glass; a glass which changes color when held up to light. The opaque green cup turns a glowing translucent red when light is shone through it. The glass contains nanoparticles of colloidal gold and silver giving it these unusual optical properties. The Lycurgus Cup is an outstanding example of this technology; its cut work and red-green dichroism render it unique.

# 2014

DIPC ACTIVITY REPORT

# Let there be Light

For millennia, men and women were surrounded by darkness.

**Physical darkness materialized every day at sunset and could only be combatted with precious firelight.** Intellectual darkness was a consequence not only of missing knowledge about the mechanisms ruling Nature but also of the lack of a proper and systematic methodology to acquire this knowledge. Moral darkness, difficult as it may be to define, was distinct in a human conscience filled with prejudices and irrationality.

Darkness prevents the full appreciation and enjoyment of the world in any of the levels mentioned above. If darkness encircles us, we cannot easily interact with our environment and we cannot identify the opportunities and threats rendered by it.

Science and knowledge provide us with light. When night falls and we turn on the lights (or now LEDs), we fight against darkness with tools designed through a long and sometimes involved process of developing scientific knowledge. When we visualize the Earth moving around the Sun at a speed of hundreds of thousands of kilometers per hour, when we turn to antibiotics to kill bacteria invading our body, or when we receive TV signals from the other side of the planet, this is illumination on our life concepts and conditions. When a democratic society freely makes a choice basing the decision on just rational and ethical arguments, this is in part a triumph of science and knowledge.

**Ricardo Díez Muiño**
Director

**Light is thus symbolic of science. But, in a more pragmatic** perspective, science uses light. Scientific practice is a technical activity in which physical light, the electromagnetic field, the sequence of photons, plays a crucial role. In physics, light is a matter of study as well as a tool used to test and probe a legion of different systems, from atoms and molecules to the latest technologically advanced bulk materials. Light-based technologies are applied everywhere, from medical therapies to communications systems, from renewable energies to the entertainment industry. It will come as no surprise then, that the UN General Assembly proclaimed 2015 as the "International Year of Light and Light-based Technologies".

Light is present in many of DIPC's lines of research. Photoemission-based techniques, attophysics, femtochemistry, photonics, laser applications, optical properties of molecules, surfaces, and nanostructures, electron dynamics, dielectric response of polymers and soft matter, nanoplasmonics, and several other topics related to the electromagnetic spectrum are current subjects of interest to DIPC scientists. At DIPC, then, we celebrate the International Year of Light doing what we have been doing for 15 years: high-level research at the frontiers of knowledge. We believe that enlarging the scientific knowledge of our society is the best way to ensure our social, cultural and economic prosperity. Scientific advances to come in the next decades will greatly change the way we live, the way we work, the way we ask questions and the finesse of the questioning. They will change the world we inhabit and they will change our culture.

**Pedro Miguel Echenique**
President

**The dim glow that our ancestors were able to keep through bonfires and torches was** carefully, almost reverentially nursed because it was instrumental in the fight against darkness. Science being one of the lights guiding humankind in its vital endeavor, it is equally important to preserve its development. Scientific research needs sustained and long-term support to progress. The knowledge so obtained is a public good in itself, but is also a necessary condition for economic growth and social progress.

Let there be science, let there be light. ■

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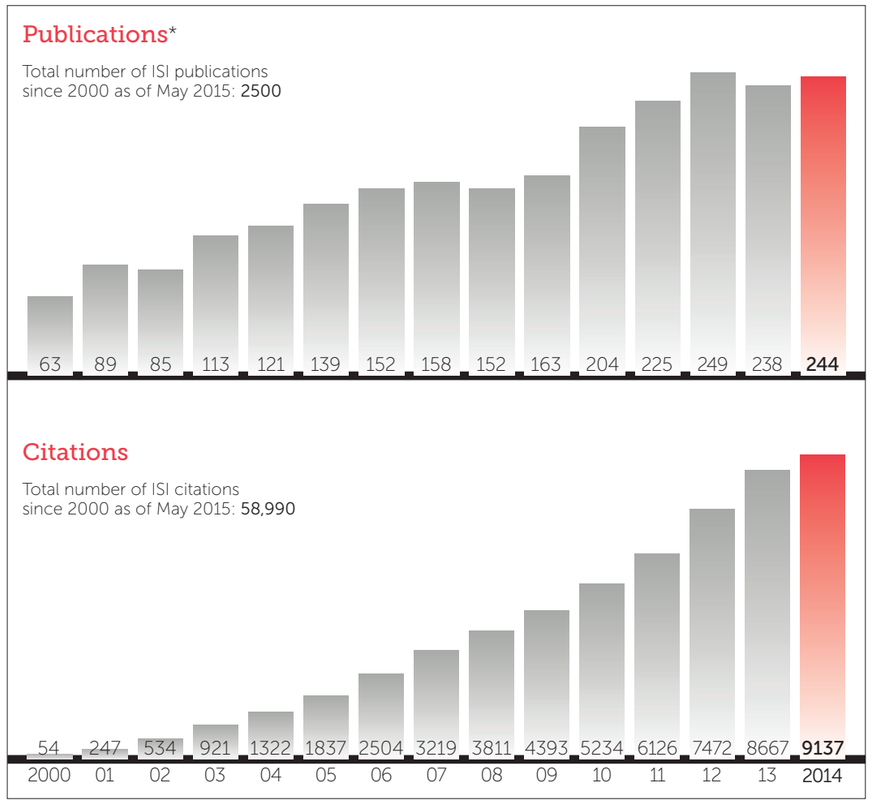
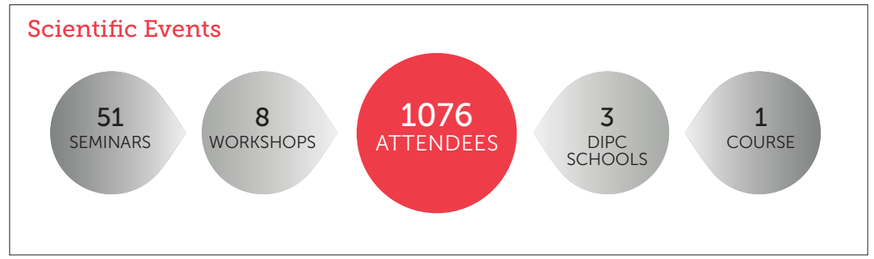
# Research Activity at a Glance

DIPC's scientific production and international impact continually increases. The center has published a total number of 2500 ISI publications. In just fifteen years since its initiation DIPC has almost quadrupled its number of publications and has received more than 58,990 citations.




*Source Web of Science Core Collection - DIPC's ResearcherID C-3171-2014 (07/05/2015)




In addition to doing research, DIPC's annual strategic agenda of actions foster exchange with scientists from around the world. Included in the program are Seminars by international experts which cover particular research topics, Workshops on specific subjects of interest, and the DIPC Schools which focus on learning particular skills.

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

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

# Science Communication

## Events dedicated to intregrating science into our society

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

### 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.

**Jean Pierre Luminet** Observatoire de Paris, LUTH, France
"Recent developments in black holes physics and astrophysics" - 30/01/2014

**Andreu Mas-Colell** Minister of Economy and Knowledge of the Government of Catalonia, Spain
"Impulsando la investigación" - 28/02/2014

**Michaela Zimmermann** Max Planck Institut, International Division Society, Münich, Germany
"Max-Planck-Gesellschaft - Measures for international cooperation" - 21/05/2014

**Manuel Aguilar Benitez de Lugo** Spanish Royal Academy of Mathematics, Physics and Natural Sciences, CIEMAT researcher and Former Vice-President of the CERN Council
"Fundamental Physics on the International Space Station" - 14/10/2014

**Luis Alvarez Gaumé** Subdirector, Division of Theoretical Physics, CERN, Switzerland
"Deconstructing Mass" - 14/10/2014

**Elena Cattaneo** Laboratory of Stem Cell Biology and Pharmacology of Neurodegenerative Diseases, University of Milan, Italy
"Huntington's Disease from evolution to pathology" - 15/12/2014

**Albert Fert** Nobel Prize in Physics 2007, Unité Mixte de Physique CNRS/Thales, France
"Spin-orbitronics, a new direction for spintronics magnetic skyrmions, spin-orbit effects in 2D electron gas at surfaces and interfaces" - 15/12/2014

### Kutxa Lectures

This series of lectures, open to the general public, started in 2010 and are organized in collaboration with Kutxa Obra Social in San Sebastian. Lecturers include top scientists and Nobel Laureates but also science communicators and humanists working in the frontiers of science. This activity addressed to citizens interested in science is an active part of the cultural life of San Sebastian. This year's events were:

**Tomás Yerro Villanueva** Public University of Navarra and Ágora Universitaria, Spain
"La Poesía a la zaga de la Ciencia" - 06/03/2014
*Included in the 4th edition of INSPIRACIENCIA, a contest for scientific inspiration stories organized by FECYT and part of the Mestizajes program* - 06/03/2014

**Giovanni Vignale** University of Missouri, USA
"Physics and Fiction: Viaje a través del alma de los físicos teóricos"- 19/06/2014

**José Ángel Martin Gago** Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain
"El origen de la vida desde la nanociencia" - 26/08/2014
*This lecture was part of the Fuerzas y Tunel 2014 Workshop.*

### New Ways of Science Lectures

A cycle of talks organized jointly by Ernest Lluch Cultural Center from Donostia Kultura and DIPC in an attempt to bring our work closer to society. Scientists from DIPC introduce the fundamentals of Material Science and historical milestones in a clear and attractive way to the general public.

**Xabier López** Chemistry Faculty, University of the Basque Country, Spain
"Bailando con proteinas" - 19/03/2014

**Jesus Ugalde** Chemistry Faculty, University of the Basque Country, Spain
"'Izarren hautsa egun batean bilakatu zen bizigai...', bai ote?" - 04/11/2014

## Celebration of CERN's 60th Anniversary

Kutxa Lecture - 14/10/2014
"60 años del CERN: Física Teórica y Grandes Experimentos"

**Manuel Aguilar Benitez de Lugo**
Spanish Royal Academy of Mathematics, Physics and Natural Sciences and Former Vice-President of the CERN Council, Spain
*Milestones of CERN during its 60 years.*

**Luis Alvarez Gaumé**
Subdirector Division of Theoretical Physics, CERN, Switzerland
*Theoretical physics developed at CERN.*

Roundtable moderated by:
**Pedro Miguel Echenique**,
President of DIPC and Professor of UPV/EHU

Mestizajes Talk at San Telmo Museoa - 15/10/2015
**Ariane Koek**
Director Arts@CERN, Switzerland
"Colliding Words - Creative Collisions Between Arts and Science"

## II Encounter on Literature and Science: Reason, Intuition and Imagination in Literature and Science

18/11/2014 and 19/11/2014

Donostia-San Sebastian, Spain
The program included a workshop aimed at specialized public at Materials Physics Center (CFM) in the mornings, and public lectures with expert from different disciplines of science and other humanities open to all citizens at Kutxa Andia Hall in the afternoons.
*See Workshops for detailed information.*

## Mestizajes

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

**Tomás Yerro Villanueva**
Public University of Navarra and Ágora Universitaria, Spain
"Poetas en la Corte de la Reina Ciencia"
Seminar at DIPC - 06/03/2014

**Ariane Koek** Director Arts@CERN, Switzerland
"Colliding Words - Creative collisions Between Arts and Science"
Seminar at DIPC and Public Lecture at San Telmo Museoa, Donostia-San Sebastian
60's anniversary of CERN - 15/10/2014

## Science Week

DIPC participated in the Science Week of the UPV/EHU along with the Materials Physics Center (CFM) and CIC nanoGUNE. On the stand "Exploring the tiny", Master's, doctorate students, and postdoctorate researchers from our centers participated in demonstrating experiments and showing young students from the local schools the fundamentals and applications of nanoscience.



## top@DIPC Encounters Zientziarekin solasean!

DIPC held the sixth edition of the Encounters between Nobel laureates and leading researchers with high school students. In these encounters, guest scientists talk about their passion for science and research and respond to questions from the students about experiences throughout their professional careers. The main objective of these encounters is to foster students' interest in scientific and technological studies and kindle a passion for knowledge in their young minds. This year's encounters in Bilbao and San Sebastian brought together students and teachers from around Euskadi.

Gran Vía BBK Hall, Bilbao - 02/10/2014
**Claude-Cohen Tannoudji**
Nobel Prize in Physics (1997)

**Juan Ignacio Cirac**
Prince of Asturias Prize for Scientific and Technical Research (2006)

*Attendance included 44 schools, 44 teachers and 137 students*

Eureka! Zientzia Museoa, Donostia-San Sebastian 15/12/2014
**Albert Fert**
Nobel Prize in Physics (2007)

**Elena Cattaneo**
Science Prize in Medicine and the Gold Medal of the Italian Republic (2001)

*Attendance included 48 schools, 49 teachers and 194 students*

## High School Visits

In 2014, for the first time, DIPC and the Materials Physics Center opened their doors to groups of high school and Baccalaureate students from around Gipuzkoa. These students had the opportunity to meet our researchers and view our work close up. This makes nanoscience and research activity real to these young minds and provides guidance and encouragement to those who are considering a career in science. During this year, 173 students and 11 teachers from seven schools in Gipuzkoa visited our center.

## Conference by Jakiunde

DIPC along with Jakiunde (Basque Academy for Sciences, Arts and Letters) organized a day dedicated to Higgs Boson. The sessions were part of the program "Krisiak 2014" by Jakiunde.

**Hegoi Garitaonaindia** CERN
"Large Hadron Collider y el detector ATLAS" - 03/04/2014
220 employees from Elay, a company that has manufactured more than 6.5 million metal parts for the Large Hadron Collider at CERN, learned about the operation of CERN and the implications of the discovery of the Higgs Boson.

**Pedro Miguel Etxenike**
President of DIPC and Professor of UPV/EHU
"De lo pequeño a lo grande. De lo simple a lo complejo. La sublime utilidad de la ciencia inútil"
*At the Town Hall of Bergara*

## ON zientzia

ON zientzia is a video contest organized yearly since 2010 by DIPC and Elhuyar Foundation, within the framework of Teknopolis, a popular TV program devoted to popularizing science and technology. The aim is to promote the production and dissemination of short, original videos on science and technology subjects. This year, the two prizes went to: Iñigo Onaindia for *JUVENA: antxoa gaztearen bila*, and Luis Navarro for *Breaking the Rules*.

# Scientifics Highlights

# Spin-dependent electron scattering at graphene edges on Ni(111)

A. Garcia-Lekue, T. Balashov, M. Olle, G. Ceballos, A. Arnau, P. Gambardella, D. Sánchez-Portal and A . Mugarza
*Physical Review Letters 112*, 066802 (2014)

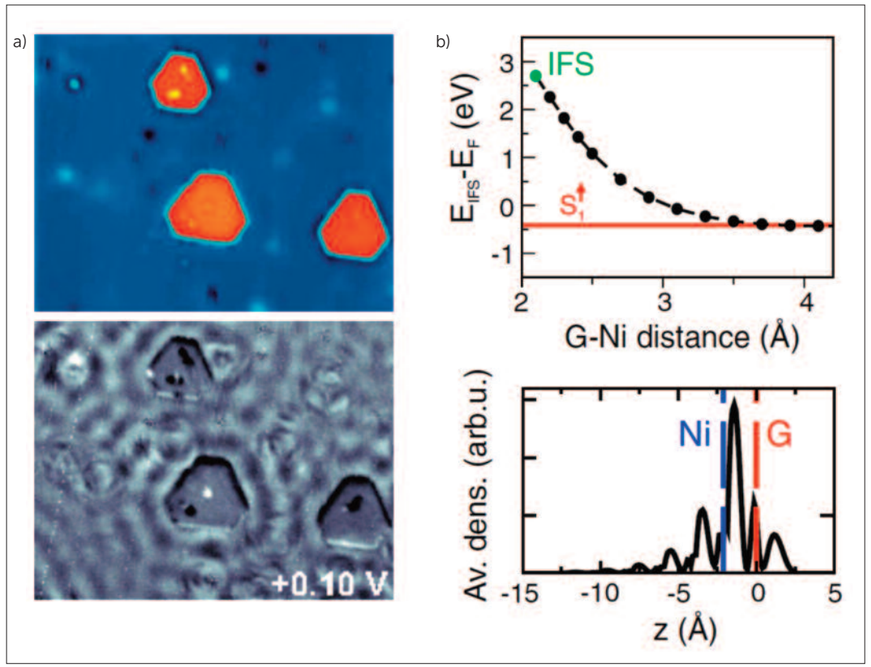
**The scattering of surface electrons by the edges of graphene islands grown on Ni(111) has been investigated by combining local tunneling spectroscopy and ab initio electronic structure calculations. We find clear signatures of spin- and edge-dependent electron scattering of the Shockley bands of Ni. Our results suggest the possibility of 2D lateral spin filtering for graphene layers, similar to that occurring across the interface.**

**The scattering of electrons** at the interface between graphene and metal contacts determines the charge and spin injection efficiency into graphene and, consequently, it is a fundamental issue for the performance of graphene-based devices. Weakly interacting metal contacts simply dope the Dirac bands. The interface with more reactive metals, however, is usually characterized by significant electronic reconstruction, which defines a complex scenario for scattering. The graphene-Ni interface represents an interesting case where the interaction with the ferromagnetic substrate opens hybridization gaps and induces magnetic moments. Consequently, graphene is predicted to behave as a perfect spin filter in contact with a magnetic Ni electrode.

In this work, we have performed a combined experimental and theoretical study of the electronic properties of graphene nanoislands with well-defined edge geometry grown on a Ni(111) substrate. The strong interaction between C and Ni atoms induces a significant energy mismatch of the surface bands inside and outside graphene, quenching the transmission through the graphene edge. This effect, together with the different coupling to bulk states of majority and minority Ni bands, leads to a spin-dependent scattering of the Shockley bands of Ni. We further demonstrate that the edge scattering is strongly structure dependent, with asymmetries in the reflection amplitude of up to 30% for reconstructed and non-reconstructed zig-zag edges.

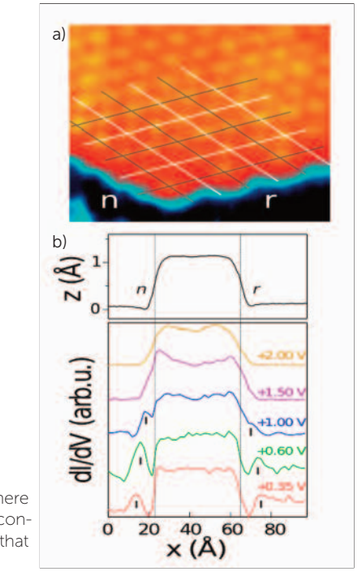
Our results elucidate the complex scattering properties of graphene-metal interfaces and are important for the control of electron transport and quantum confinement in lateral graphene junctions with spin-polarized electrodes.

## Unraveling the complex scattering properties of graphene/metal interfaces




(a) Topographic ($V_b$ = 0.1V) and constant current dI/dV map showing the interference pattern of the $S_1$ surface state scattered from graphene islands. Setpoint current: I = 0:3 nA. Image size: 30 x 37 $nm^2$. (b) Top: calculated energy of the majority interface states (IFS) as a function of the distance between the graphene layer and the Ni surface. The energy of the S1 surface state for pristine Ni(111) is represented by the red line. Bottom: electron density associated with the majority IFS averaged over a plane at the equilibrium distance (2.1Å).

## Scattering of spin-split surface states at graphene edges: lateral spin filtering effect




(a) Atomically resolved topographic image of a graphene island, where reconstructed edges (r) exhibit twice the periodicity of the nonreconstructed ones (n). (c) Topographic dI/dV profiles taken along a line that crosses the graphene island.

# Co nanodot arrays grown on a $GdAu_2$ template: Substrate/nanodot antiferromagnetic coupling

L. Fernández, M. Blanco-Rey, M. Ilyn, L. Vitali, A. Correa, P. Ohresser, E. Ortega, and A. Ayuela, F. Schiller
*Nano Letters 14,* 2977 (2014)

**Controlling anisotropy and exchange coupling in patterned magnetic nanostructures is key to develop advanced magnetic storage and spintronic devices. We report on the antiferromagnetic interaction between a Co nanodot array and its supporting $GdAu_2$ nanotemplate that induces large anisotropy values in individual Co nanodots. In clear contrast with nonmagnetic Au substrates, $GdAu_2$ triggers an earlier switch from out-of-plane anisotropy in atomic high dots to in-plane when the dot height becomes biatomic.**

## Playing with nanomagnets at the interface: the role of rare earth atoms

One of the biggest challenges in magnetic storage and spintronics is to fabricate arrays of magnetic nanodots. On the one side, the objective is to achieve the densest network made of independent magnetic nanoelements, and on the other side the objective is to develop functional interfaces for spintronics. Here, we address the characterization of a periodic Co nanodot array self-assembled on a ferromagnetic (FM) nanotemplate of $GdAu_2$[1,2]. This article deals with the fundamental question about the nature of the anisotropy and magnetic coupling across the interface between the nanostructures and the template.

## Substrate/nanodots antiferromagnetic coupling

We focus the present study on arrays of independent Co nanodots on a monolayer thick $GdAu_2$ surface compound, where two different types of dots are observed being one or two atomic layer (AL) heights (see Figure 1). The magnetic response of the Co nanodot array is shown in Figure 2 through element-specific X-ray magnetic circular dichroism (XMCD) analysis taken at the DEIMOS beamline. The shape of the XMCD asymmetry spectra is inverted with respect to the Gd atoms of the substrate indicating antiferromagnetic (AFM) coupling. Magnetization loops taken on the Co $L_3$ and the Gd $M_5$ absorption edges confirmed the AFM interaction and evidence a strong coupling. This is certified by our full-potential linearized augmented plane waves (FLAPW) calculations within the density functional theory (DFT) that probe the exchange coupling between Co and Gd. The systems are modeled by periodically ordered Co atoms and overlayers in contact with a free standing $GdAu_2$ monolayer. Starting from the calculated adsorption energies we can estimate the critical magnetic field $H_{cr}$ to overcome the AFM coupling between Co and $GdAu_2$. $H_{cr}$ is found to be of 1000 T for single Co atoms, while in the case of 1 monolayer (ML) it reduces to 100 T. For 2ML and 3ML, $H_{cr}$ is about 10 T.

[1] M. Corso et al. ACS Nano 4, 1603 (2010).
[2] L. Fernández et al. Appl. Phys. Lett. 96, 013107 (2010).





## Magnetic anisotropy energy

The magnetic anisotropy was probed using different sample geometries with respect to the magnetic field and to the photon propagation vector. We found a reduction of the strong in-plane anisotropy of the $GdAu_2$ substrate after Co dot adsorption (see Figure 3). Such a situation occurs if the dots reveal an out-of-plane anisotropy. This is again ratified by the DFT calculations. Clean $GdAu_2$ layers have magnetic anisotropy energy (MAE) of 2.7meV per unit cell and show an in-plane easy-axis of magnetization. Moreover, the magnetic anisotropy of Co grown on $GdAu_2$ layers is found to be strongly dependent on Co coverage. Up to 1 AL thick Co dots the easy axis is perpendicular to the surface. In contrast, for more than 2 AL the easy-axis changes to in-plane. The magnetization curves of Figure 3 suggest that upon adsorption of 1 AL Co nanodots, a local out-of-plane anisotropy reorientation takes place in the underlying $GdAu_2$ alloy.

In conclusion, experiment and theory demonstrate the strong AFM coupling between Co and Gd. The electronic interaction between Co dots and substrate induces significant changes on the Co anisotropy, leading to a switch from out-of-plane for monoatomic high dots to in-plane easy axis direction in biatomic high Co dots. Given the variety of the rare earth-noble metal moiré templates, the present study opens up a new route to explore similar magnetic nanodot arrays on different RE-$Au_2$ surfaces.

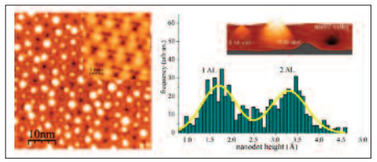



Figure 1. (a) Self-organized Co nanodots on $GdAu_2$ (0.6ML). The inset shows the $GdAu_2$ template. (b) Histogram with nanodot height distribution. The inset displays one and two AL height nanodots together with a moiré minima.

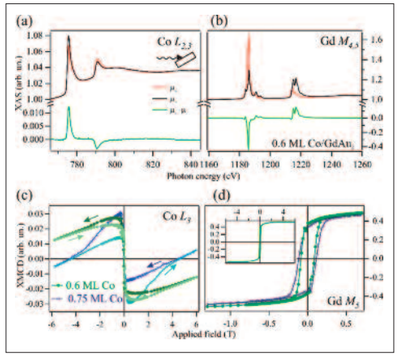



Figure 2. XAS measurements of 0.6ML Co/ $GdAu_2$ measured at 3K with an applied magnetic field of 6T and θ=60° incidence from: (a) Co at the $L_{2,3}$, and (b) Gd at the $M_{4,5}$ absorption edges. (c,d) XMCD asymmetry signals as a function of applied field for 0.6 and 0.75ML Co on $GdAu_2$, respectively.

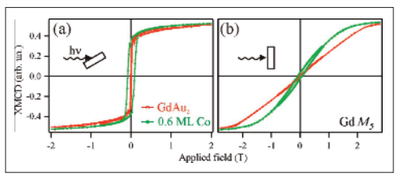



Figure 3. XMCD element specific magnetization curves measured at the Gd M5 absorption edge from Co free and Co covered $GdAu_2$ layers (T=3K) at (a) in-plane, and (b) out-of-plane geometry, respectively. The clean substrate loops indicate FM Gd with large uniaxial, in-plane anisotropy.

# Electronic friction dominates hydrogen hot-atom relaxation on Pd(100)

M. Blanco-Rey, J. I. Juaristi, R. Díez Muiño, H. F. Busnengo, G. J. Kroes and M. Alducin
*Physical Review Letters 112*, 103203 (2014)

**The dynamics of hot H atoms propagating on a Pd surface has been investigated by a newly developed methodology, AIMDEF. This study shows that the electronic effects dominate the energy exchange between the H atoms and the surface.**

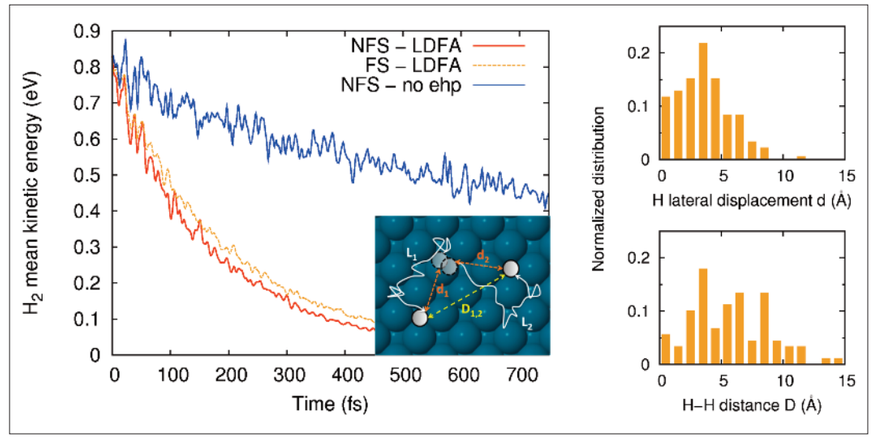
**The performance of a material** under realistic working conditions is highly dependent on the way it interacts with its environment. For this reason, the study of solid surfaces at the atomic scale is one of the most active fields of research in materials science. One of the current challenges is the modelling of the interaction dynamics between gas-phase atoms or molecules and a surface. The so-called ab-initio theoretical methods have contributed many advances in this field over the last few decades.

An important question is how energy is dissipated during the interaction time, i.e. how the gas species xchanges energy with the surface. This issue may have implications for the chemical properties of the surface or for its durability, in the case the surface is to be used as a catalyst or a coating. Even in apparently simple cases, such as an atom interacting with a metal, it is difficult to describe the gas/solid interaction processes, since many parameters come into play: chemical reactivity of the surface, momentum of the approaching species, surface temperature, etc.

Researchers of the DIPC and the CFM have investigated by means of ab-initio simulations the fate of a $H_2$ molecule that dissociates upon impact on a Pd surface. The energy contained in the molecular bond (a few eV) is liberated and, as shown by the simulations, the resulting H atoms initially acquire considerable propagation velocity on the surface. These "hot" H atoms slow down by transferring their kinetic energy to the Pd substrate using two channels: motion of the Pd nuclei via H-Pd collisions and electronic excitations of the metal surface charge. It was thought so far that the former channel was dominant for H on Pd, but this investigation has determined that the electronic channel can in fact decelerate the hot atoms at a five times larger rate, as shown in the Figure.

This finding could not have been accomplished without improving the existing theoretical methods with the inclusion of electronic excitations. These are accounted for "on-the-fly" at each point of the trajectory followed by the hot atom as a friction force that opposes its movement. The strength of this force depends on the charge density of the metal at each position, which is known as the LDFA approach. This technique has been denoted with the acronym AIMDEF (ab-initio molecular dynamics with electronic friction).

It is worth noting that this result for hot H atoms on Pd is compatible with the experimental observation of chemicurrents, i.e. electric currents that originate during adsorption, dissociation and recombination of a molecule on a metal. Chemicurrents may be used as sensors of chemical processes, and the deceleration rates found by AIMDEF can help calibrate them. In addition, AIMDEF demonstrates that energy dissipation happens gradually during the hot species propagation on the surface, rather than instantaneously. The simulations also yield the distances travelled by the hot atoms (see Figure) before stopping. Thus, it can be predicted whether the transient species can jump into and recombine with other species on the surface. Since the travelled distances cannot be inferred from the energy dissipation rate values alone, AIMDEF comes in as a valuable tool to characterise the chemical activity of the surface, too.




Results for a $H_2$ molecule incident on a Pd(100) surface with 0.5 eV. Left panel: evolution in time of the $H_2$ kinetic energy after bond breaking. (N)FS stands for (non-) frozen surface atoms during the simulation. The blue line is the result for no electronic excitations. Inset: artist's view of the erratic trajectories followed by the dissociation products. Right panel: distributions of the travelled parallel distances depicted in the inset for the FS – LDFA case.

## Electronic brakes for hot atoms travelling on a metal surface

# Self-assembly of bicomponent molecular monolayers: Adsorption height changes and their consequences

E. Goiri, M. Matena, A. El-Sayed, J. Lobo-Checa, P. Borghetti, C. Rogero, B. Detlefs, J. Duvernay, J. E. Ortega, and D. G. de Oteyza
*Physical Review Letters 112*, 117602-1-5 (2014)

**Surprising changes in the adsorption heights of molecules within donor-acceptor monolayer blends are found to have a measureable effect on the system's interface dipole.**

**Charge carrier injection in organic optoelectronic devices** depends on the electronic properties of metal-organic interfaces, which are, therefore, of utmost importance for device efficiency. Such properties are strongly affected by the detailed interfacial structure defined by the molecular orientation with respect to the substrate, the lateral distribution, and the molecule-substrate distance. The latter, in particular, plays a central role in the interfacial energy level alignment due to of its interrelation with the interface dipole.

The most precise technique to determine the molecule-substrate distance experimentally is normal incidence x-ray standing waves (XSW). In this work we go beyond the common characterization of single-component layers, using XSW for the first time to determine molecule-substrate distances in donor-acceptor molecular blends, which hold particular interest for many organic devices.

We focus on the characterization of donor-acceptor blends comprising copper-phthalocyanines (CuPc, donor) and perfluoropentacene (PFP, acceptor). The lateral order of the 2D blends and the molecule-substrate distances have been acssessed using scanning tunneling microscopy (STM) and XSW, respectively. Electronic properties have been investigated by photoemission. STM measurements show that codepositing CuPc and PFP on Ag(111) and Cu(111) leads to the self-assembly of ordered molecular layers in which molecules adopt a flat-lying configuration. As shown in Figure 1, donor-acceptor contact is maximized in the layers, thereby optimizing C-H···F intermolecular hydrogen bonds.

Regarding the adsorption heights of CuPc and PFP we find that, as compared with single-component layers, the PFP-substrate distance increases by ~0.3 Å in the blends. Instead, CuPc shows only negligible changes. Figure 2 shows a schematic of adsorption heights of CuPc and PFP in single component and mixed layers, evidencing how PFP's surprising adsorption height change further increases the height difference between neighboring molecular species in the blend. The changes in adsorption height found in the mixed layer are expected to lead to variations in the interface electronic properties. Indeed, work function measurements on the mixed layers show that PFP's contribution to the interface dipole is reduced by about 40% with respect to what would be expected from its configuration in the single-component layer. We argue that the increased molecule-substrate distance of PFP found in the mixture translates into a reduced Pauli repulsion, thereby decreasing the effective interface dipole. We hereby provide a direct measure of the effect of a molecule's adsorption height on vacuum level shifts and, in turn, interfacial energy level alignment.

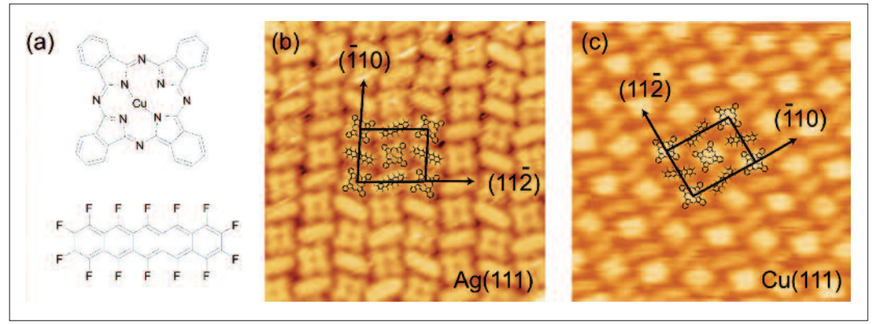



Figure 1. (a) Chemical structure of CuPc (above) and PFP (below). (b) and (c) 11.5 nm ×11.5 nm images of the 1:1 PFP+CuPc blend on Ag(111) and Cu(111), respectively.

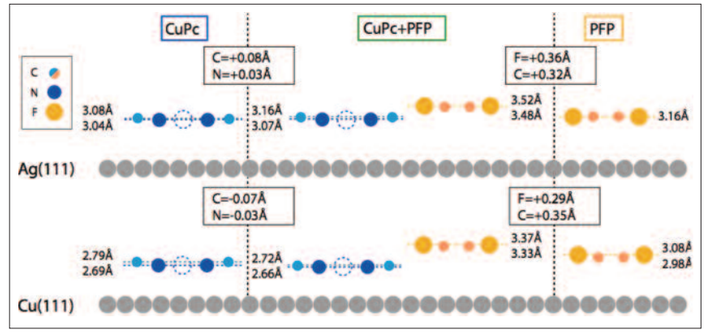



Figure 2. Molecular adsorption heights of CuPc monolayers (left), PFP monolayers (right), and the PFP+CuPc mix (center) on the Ag(111) (top) and Cu(111) (bottom) surfaces, including height changes in the mixed layers referred to the single-component monolayers. Distance to the substrate is not to scale. Monolayer data is taken from the literature.

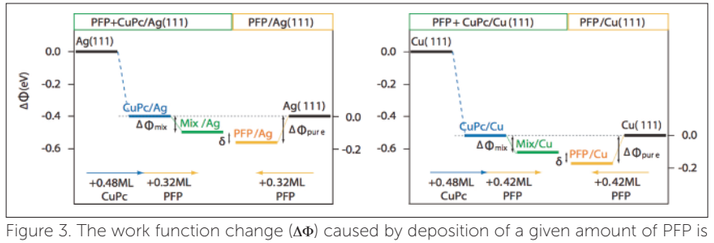



Figure 3. The work function change (ΔΦ) caused by deposition of a given amount of PFP is reduced by an amount δ when PFP is deposited upon a precovered submonolayer CuPc=metal system (ΔΦmix), as compared to deposition on the clean metal (ΔΦpure). The effect is observed on both Ag(111) (left) and Cu(111) (right). The blue bar (CuPc=metal) and the black bar (clean metal) have been aligned in order to more easily compare ΔΦmix and ΔΦpure.

# Chemical control of electrical contact to $sp^2$ carbon atoms

T. Frederiksen, G. Foti, F. Scheurer, V. Speisser and G. Schull
*Nature Communications 5,* 3659 (2014).

**Research carried out at UPV/EHU, DIPC and CNRS advances the understanding of electric contacts in future carbon-based nanoelectronics.**

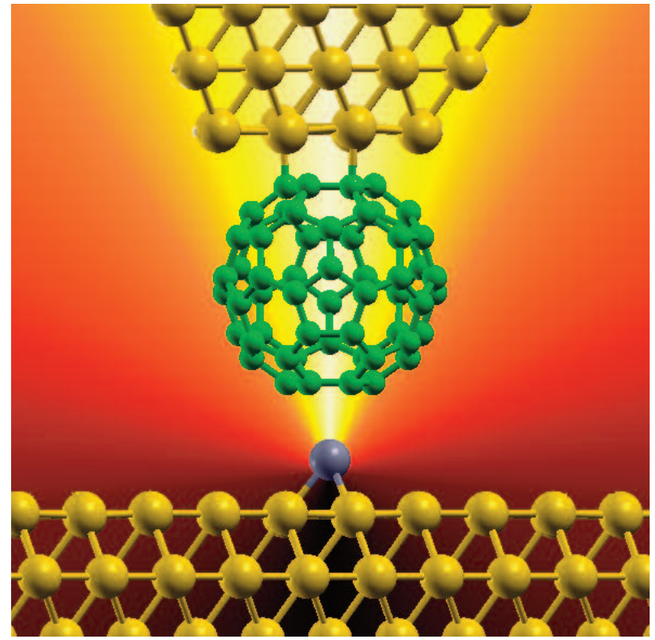
**Carbon-based nanostructures** such as nanotubes, graphene sheets, and nanoribbons are unique building blocks showing versatile nanomechanical and nanoelectronic properties. These materials which are ordered in the nanoscale, that is, in the dimension of a millionth of millimetre, are promising candidates to envision applications in nanoscale devices, ranging from energy conversion to nano-electronic transistors. A good connection between carbon-based materials and external metallic leads is of major importance in nano-device performance, an aspect where an important step has been surmounted by researchers from UPV/EHU, DIPC and CNRS by studying contacts of carbon nanostructures with atoms of different chemical nature.

The chemical nature of contacting leads is of major importance as it affects the electronic properties and the geometry of the contact. The impact of these two aspects on the transport properties are entangled and this group studied these two parameters for contacts shrunk to the limit of individual atoms as for large structures it is challenging to address them separately.

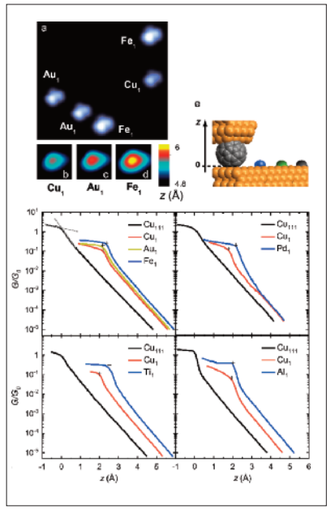
In close collaboration, the researchers used a prototype carbon-based molecule made of 60 carbon atoms arranged in a sphere that can be viewed as a graphene sheet rolled into a tiny ball. The experimental team in Strasbourg led by Guillaume Schull, attached this molecule to the apex of an extremely tiny metal needle of a scanning tunnelling microscope (STM). The molecule-terminated needle was then cautiously approached to individual metallic atoms of different chemical nature up to the formation of a robust connection. By simultaneously measuring the electrical current passing through these connections, they could deduce which of the individual metallic atom is injecting charges to the carbon-made molecule with the greatest efficiency.

Large-scale computer simulations performed by the theoretical team in San Sebastian led by Thomas Frederiksen, Ikerbasque Research Professor at the DIPC, revealed a fascinating and unexpected aspect of these extremely tiny connections: their electric and mechanical properties are in fact representative for much larger carbon-based materials.

These results, published in the prestigious journal *Nature Communications*, set the bases to find extremely efficient contacts in the near future. The study paves the way to probe a great number of different metallic species (as well as tiny alloys made of two or three different metallic atoms), allowing for a systematic classification of their abilities to inject electrons into emerging carbon-based electronic devices.



Artistic view of an electric connection between a $C_{60}$ molecule (attached to the tip of a STM) and a single metallic adatom (gray ball). The researchers were able to quantify how the current depends on the chemical nature of the contacting adatom.




## A small connection with big implications: Wiring up carbon-based electronics

Individual metal adatoms contacted with a $C_{60}$-functionalized STM tip. (a) STM image (7.0 × 6.2 $nm^2$) of different metal adatoms on Cu(111) acquired with a C60 tip at a sample voltage $V$ = 1.7 V. (b–d) Close-up views (1.4 × 1.4 $nm^2$) of $Cu_1$, $Au_1$ and $Fe_1$ images with a $C_{60}$ tip for tunnelling conditions corresponding to the initial parameter of the traces in f. (e) Sketch of the $C_{60}$ tip where z = 0 corresponds to contact with the flat surface. (f) Experimental conductance traces *G(z)* in units of the conductance quantum $G_0 = 2e^2/h$. Black crosses mark the contact points defined as the intersection of the contact and transition regimes such as indicated by the dashed grey lines in panel f for the bare surface data.

# Time-resolved random laser spectroscopy of inhomogeneously broadened systems

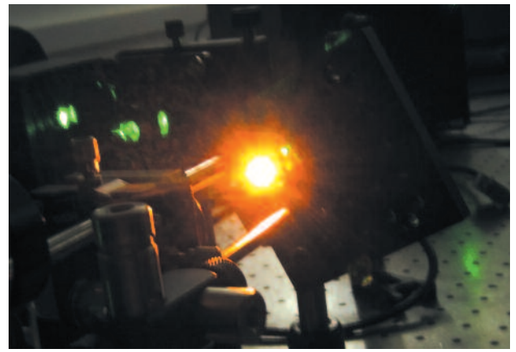
J. Fernández, S. García-Revilla, L. D. Carlos, E. Pecoraro, M. A. Arriandiaga and R. Balda
*Laser and Photonics Rev. 8*, No. 3, L32-36 (2014)

**The understanding of energy transfer processes in biological systems occurring among optical centers which exhibit inhomogeneously broadened spectral bands is of paramount importance to determine time constants and spatial distribution of energy flow. In this work a new time resolved-spectroscopy based on the random laser generation of the optical probes is reported. This new spectroscopy may resolve not only the spectral features of the system but also provide a high speed picture of the energy transfer and excited state relaxation of efficient interacting chromophore pairs embedded in inhomogeneous scattering structures.**

**It is well known that in fluorescence,** much of the molecular information content is available only by time-resolved measurements. Frequently, macromolecules can exist in more than a single conformation, and the decay time of a bound probe may reveal the presence of different conformational states. Moreover, in the presence of energy transfer, the intensity decays map out the rate of the process and may provide information about the excited-state dynamics of both donors and acceptors. Among time-resolved spectroscopies, fluorescence line-narrowing is one of the most suitable for studying interline energy transfer in inhomogenous broadened systems. The measurements are made at low temperature, where kT is much less than the chromophore spectral width. In spite of this, the theoretical grounds of such spectroscopy can be applied to the dynamics of the room temperature excited state of an inhomogeneously broadened transition when the excited state is followed by its own random laser emission produced by multiple light scattering. The random laser process selects only a small subset of emitting centres which gives the well known narrowed spectral emission.

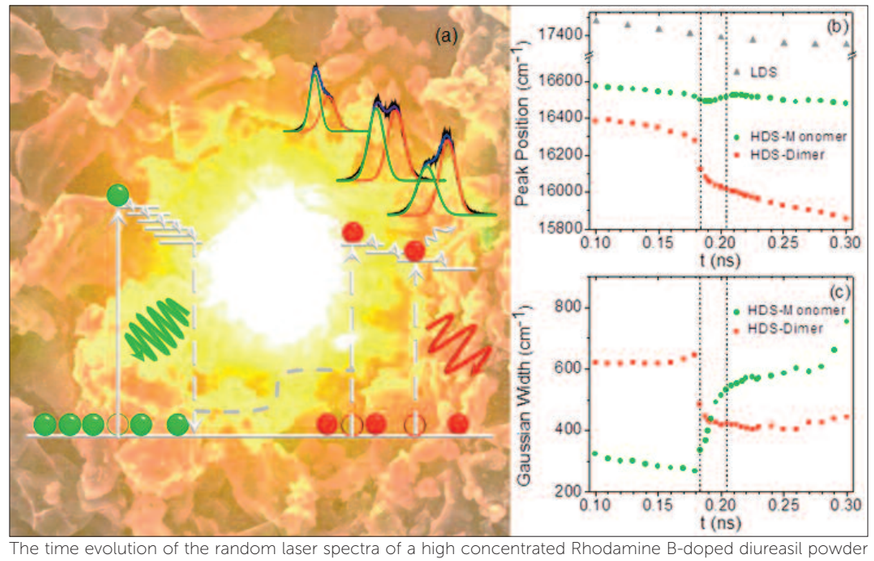
In this paper, scientists from DIPC explore the potentialities of random lasing as a spectral probe of molecular relaxation in high concentrated Rhodamine B-doped d-U(600) organic-inorganic diureasil hybrid powders. The analysis of the random laser emission, which was detected by using a streak camera, shows that the energy transfer between Rhodamine B monomers and dimers is at the origin of random laser emission of dimer species and can be formally interpreted as spectral migration in a similar way to fluorescence line narrowing in inhomogeneously broadened systems. It is worth noticing that in spite of the overlapping between the emission bands of monomers and dimers, the frequency selection introduced by the random laser process allows to discriminate from both groups of emitters. Moreover, the subnanosecond nature of the random lasing buildup time allows for a real time tracking of the transfer process between them.

This new random lasing-based spectroscopy can, in principle, be applied to any kind of efficient interacting chromophores pairs and could efficiently help to understand the spectro-temporal dynamics of ultrafast energy transfer processes occurring at cellular level, when engineered efficient chromophore markers are used as sensors. The results open a new door for the application of random laser emission in complex systems and provide a new tool for high resolution studies of spectro-temporal energy transfer processes at room temperature.



Photograph of the random laser emission of a high concentrated Rhodamine B-doped diureasil powder.

A new random laser based spectroscopy is reported.




The time evolution of the random laser spectra of a high concentrated Rhodamine B-doped diureasil powder (HDS) resembles an energy transfer mechanism in which the excited state population of monomers loses its energy by fast nonradiative processes populating the excited state of dimers with lower lying energy levels. The frequency selection introduced by the random laser process allows to discriminate the emissions from both groups of emitters and to follow the energy transfer process between them in real time (a). Time dependence of the monomer and dimer emission peaks (b) and of the corresponding spectral widths (c) obtained from the fits to the sum of two Gaussians of the time resolved emission spectra of the heavily doped sample (HDS). Grey triangles in (b) show the time dependence of the single peak of a low Rhodamine B-doped sample (LDS).

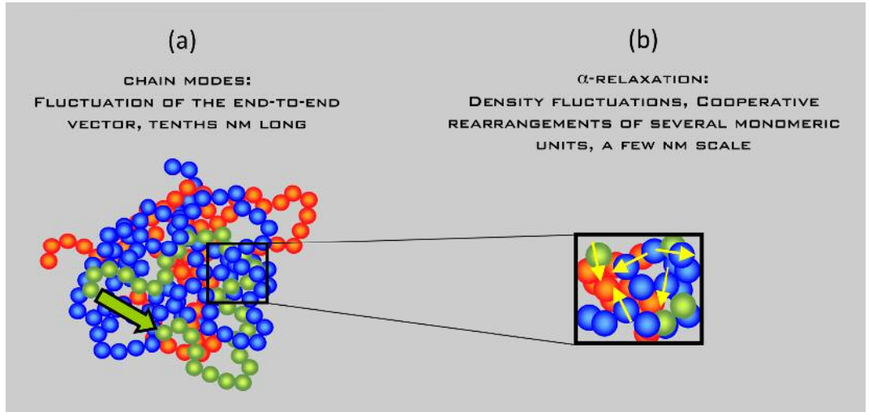
# Polymer chain dynamics: Evidence of nonexponential mode relaxation using thermally stimulated depolarization current techniques

S. Arrese-Igor, A. Alegría, and J. Colmenero
*Physical Review Letters 113,* 078302 (2014)

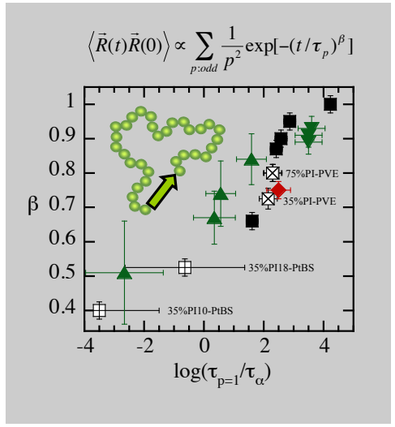
**Actual theories for macromolecular chain dynamics assume exponential relaxation for the different chain modes while molecular dynamics simulations usually show deviations from the exponential behavior. In this work thermally stimulated depolarization current technique was used to show that on approaching the range of the kinetic glass transition the slowest (p=1) chain mode significantly deviates from an exponential decay.**

**Fluctuations of the end-to-end vector of a polymer chain** are at the basis of the viscoelastic properties having thus great impact on the processing and final application of macromolecular systems in general. Although molecular dynamics simulations usually show deviations from the exponential behavior, actual theories for macromolecular chain dynamics assume exponential relaxation for the different chain modes, i.e. the spatial and time correlations of the random forces acting on a polymer segment are neglected. Testing the question from an experimental point of view however has remained elusive due to difficulties in recording the response of a single mode rather than the global response (addition of several modes).

In this work the authors have developed an experimental procedure to isolate the slowest chain mode (p=1) relaxation by means of thermally stimulated depolarization current (TSDC) technique. It has been shown that on approaching the range of the kinetic glass transition ($T_g$) the relaxation p=1 mode significantly deviates from an exponential decay, i.e., from the behavior assumed by Rouse and tube-reptation theories. The effect is found to be more pronounced the closer the timescale of the p=1 chain mode and that of the local density fluctuations ($\alpha$-relaxation) leading to the glass transition process. The observed behavior is consistent with an scenario where exponentiality for the chain modes would be lost as a consequence of breaking the condition of time uncorrelation for the forces acting on a chain segment due to the slowing down of the local density fluctuations. Moreover, the phenomenology observed for homopolymers close to the glass transition resembles that observed for the chain dynamics of the fast component in blends with high dynamic asymmetry when approaching the glass transition of the slow component, and suggests a general interpretation for both contexts.




Schematic representation of the length scales involved in density fluctuations leading to the $\alpha$-relaxation (a) and fluctuations of the end-to-end vector (b).




Parameter $\beta$ describing the non-exponential character of the mode relaxation as a function of the ratio between the timescales of the slowest (p=1) chain mode and the relevant density fluctuations in the system (the $\alpha$-relaxation in the case of homopolymers and the $\alpha$-relaxation of the slow component in the blends): linear polysioprenes of different molecular weights by TSDC (black squares); linear polyethyleneglycol by TSDC (red diamond); linear polyisoprene –fast component– blended with higher $T_g$ PtBS and PVE –slow components– by TSDC (white squares); linear polyethyleneoxide by MDS (downside triangles); and 20% linear polyethyleneoxide –fast component– blended with higher $T_g$ polymethylmethacrylate –slow component– by MDS.

The exponential character of the slowest chain mode relaxation is lost as a consequence of breaking the condition of time uncorrelation for the forces acting on a chain segment due to the slowing down of the local density fluctuations.

# Determining the polarization state of an extreme ultraviolet free-electron laser beam using atomic circular dichroism

T. Mazza, M. Ilchen, A.J. Rafipoor, C. Callegari, P. Finetti, O. Plekan, K.C. Prince, R. Richter, M.B. Danailov, A. Demidovich, G. De Ninno, C. Grazioli, R. Ivanov, N. Mahne, L. Raimondi, C. Svetina, L. Avaldi, P. Bolognesi, M. Coreno, P. O'Keeffe, M. Di Fraia, M. Devetta, Y. Ovcharenko, Th. Möller, V. Lyamayev, F. Stienkemeier, S. Düsterer, K. Ueda, J.T. Costello, A.K. Kazansky, N.M. Kabachnik and M. Meyer
*Nature Communications 5*, 3648 (2014)

**Two-color photoionization of an atom is a powerful and straightforward tool to determine the sign of the helicity and the magnitude of circular polarization of any XUV or indeed X-ray FEL beam with high accuracy. Moreover, this study confirms the theoretical prediction of CD in the two-color multi-photon ionization of atoms.**

**Ultrafast extreme ultraviolet and X-ray free-electron lasers** are set to revolutionize many domains such as bio-photonics and materials science. These short-wavelength FELs enable investigation of non-linear phenomena and femtosecond time-resolved spectroscopy. In addition, X-ray FELs have enabled imaging experiments aiming to determine the structure of a single biomolecule.

Nearly all short-wavelength FEL experiments to date have been carried out with linearly polarized light. As far as we know, only one experiment was performed with circularly polarized light but at the expense of a strong reduction in intensity. This limitation was overcome only recently thanks to FEL FERMI, designed specifically to produce circularly polarized extremely intense XUV radiation.

In this work, polarization properties of FEL beam were studied using circular dichroism (CD), a phenomenon that in photoemission is defined as the difference of the photoelectron yield for left and right circularly polarized ionizing radiation. In the experiment (Figure 1), He atoms were ionized by XUV FEL radiation which was kept fixed (left-handed circular) in the presence of an intense-near infra red (NIR) laser field which was switched from left- to right handed polarization.

Characterization of the polarization properties of the FEL beam was carried out by analyzing the sidebands in the photoelectron spectrum and compared with theory (Figure 2):
• Maximal electron emission observed at 90° is in agreement with theoretical results.
• The angular distribution with two sidebands (caused by a two-photon process) is much narrower than that of the 1 s photoline (mostly from a one-photon process).
• Dichroism of opposite sign for the main line and the sidebands is observed both for experiment and theory.

The observation of the CD demonstrates unequivocally that chirality is introduced into the (initially unpolarized atomic) system by the circularly polarized ionizing XUV radiation. The overlap with an NIR-dressing field of the same or the opposite helicity causes different probabilities for the transfer of electrons from the main line to the sidebands, i.e., for the free-free transitions.

The degree of circular polarization is obtained by comparing the CD determined from the experimental and the simulated theoretical electron spectra at emission angles of (90±4)°, where theory predicts maximal CD.
• Measured amplitude of the CD is 0.04±0.004 at the high-energy sideband (25.2–26.1 eV).
• Pcirc=0.95±0.05 for the XUV radiation.

CD measurement is in excellent agreement with theory and Pcirc with predictions. The method is therefore an important metrological tool for the determination of the degree of circular polarization, which is otherwise difficult to measure at the high power levels used here. Moreover, the sign of the dichroism is directly related to the relative helicity of both the NIR and XUV fields; the negative dichroism indicates that the FEL beam was in a state of left-handed circular polarization.

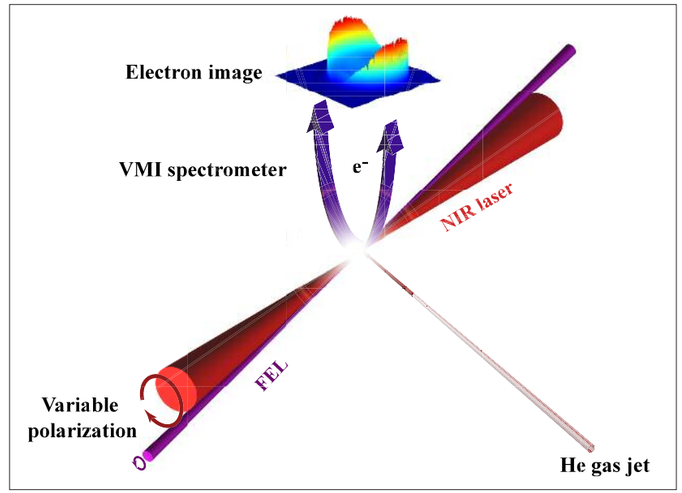
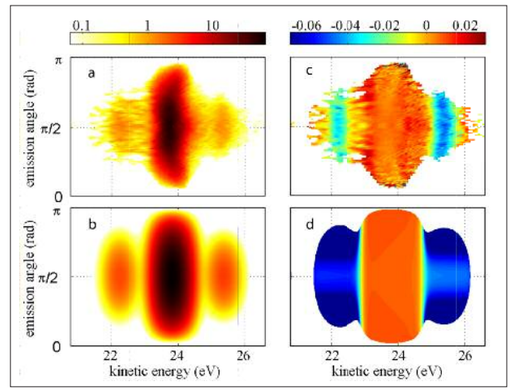


Figure 1. Experimental setup used at the low density matter (LDM) end-station of FERMI.

Figure 2. Angle and energy-resolved electron spectra and circular dichroism. Double differential cross section (a,b) and differential circular dichroism (c,d) in H2 1s photoionization. (Experimental results in the upper pannels and simulations in the lower panels.)



DIPC HIGHLIGHT 2014

# Epitaxially connected PbSe quantum-dot films: Controlled neck formation and optoelectronic properties

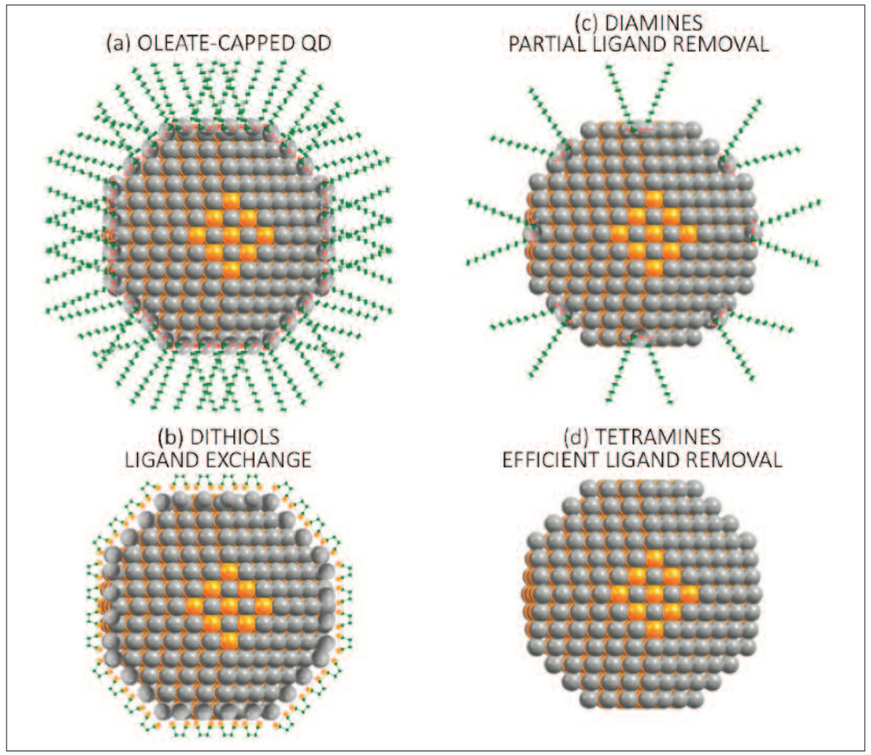
C.S. Suchand Sandeep, J. M. Azpiroz, W. H. Evers, S. C. Boehme, I. Moreels, S. Kinge, L.D.A. Siebbeles, I. Infante, A. J. Houtepen
*ACS Nano, 8(11)*, 11499-11511 (2014)

**Currently, silicon-based single-junction solar cell devices available in the market have a reasonable efficiency of 15% but they suffer of high production cost. To increase the efficiency and lower the costs, a new generation of solar devices based on nanomaterials is being developed. Quantum dots solar cells (QDSC) are among these most promising new photovoltaic cells and in just few years they passed from efficiencies below 1% to almost 10%.**

**Quantum dots (QDs) are semiconductor nanocrystals** that present very fascinating properties like high extinction coefficients, a tunable bandgap with size, carrier multiplication and also hot carrier extraction. When QDs are placed on a thin film and then photoexcited, the generated holes and electrons are extracted at two different electrodes to generate current. One of the main problems of this cell is that electron and holes can recombine before reaching the electrodes. This creates short-circuits, lowers the diffusion length of the film and reduces the device performance. To circumvent these problems, it is paramount to increase electron-hole mobility.

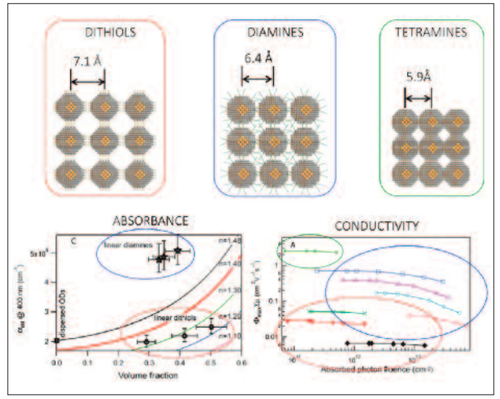
In this work, we have collaborated with the optoelectronic group at TU Delft in the Netherlands to combine theoretical calculations based on Density Functional Theory (DFT) with experiments. Ligand exchange is a much-used method to increase the conductivity of colloidal QD films by replacing long insulating ligands on QD surfaces with shorter ones. Here we show that while some ligands indeed replace the original ones as expected, others may be used to controllably remove the native ligands and induce epitaxial necking of specific crystal facets. In particular, with our DFT calculations, we have demonstrated that amines strip lead oleate from the (100) surfaces of PbSe QDs. This leads to necking of QDs and results in cubic superlattices of epitaxially connected QDs. The number of amine head-groups as well as the carbon chain length of linear diamines is shown to control the extent of necking. DFT calculations show that the removal of Pb(oleate)2 from (100) surfaces is exothermic for all amines, but the driving force increases as monoamines < long diamines < short diamines < tetramines. The neck formation and cubic ordering results in a higher optical absorption cross section and higher charge carrier mobilities, thereby showing that the use of the proper multidentate amine molecules is a powerful tool to create supercrystals of epitaxially connected PbSe QDs with controlled electronic coupling.

In summary, our DFT calculations have been used as a powerful tool to identify organic ligands that ultimately led to a 5-fold increase in conductivity of PbSe QD films. These novel films can be ultimately exploited to increase the efficiency of solar devices.




Atomic structure of the native oleate-capped PbSe QDs (a), and of those treated with dithiol (b), diamine (c), and tetramine (d) ligands. Notice that dithiols induce ligand exchange, while amines produce ligand removal.

QD films treated with dithiol (red), diamine (blue), and tetramine (green) ligands. Note that the optical absorbance and the electrical conductivity improve with the compactness of the film.




Our DFT calculations have been used as a powerful tool to identify organic ligands that ultimately led to a 5-fold increase in conductivity of PbSe QD films.

DIPC HIGHLIGHT 2014

# Complex chiral colloids and surfaces via high-index off-cut silicon

K.M. McPeak, C.D. van Engers, M. Blome, J.H. Park, S. Burger, M.A. Gosalvez, A. Faridi, Y.R. Ries, A. Sahu, and D.J. Norris
*Nano Letters 14*, 2934 (2014)

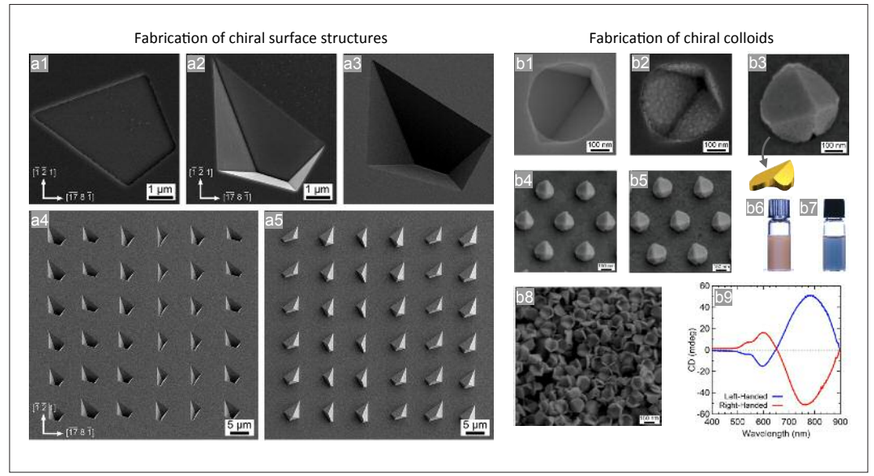
Highly symmetric surface cavities are commonly obtained on masked silicon wafers through selective exposure of circular and polygonal areas to alkaline solutions. The cavities arise because the silicon {111} atomic planes are etched slowly, compared to any other crystallographic orientation. We apply this traditional etching technique to nonstandard, high-index, off-cut silicon {137} wafers, resulting in the generation of highly complex, nanoscale, chiral cavities that would otherwise be difficult to produce. By using such cavities as templates where metals such as Ag or Au can be deposited, the study demonstrates the production of chiral gold surfaces and nanoparticles of a specific handedness. When the nanoparticles are dispersed in liquids, gold colloids exhibiting record molar circular dichroism at red wavelengths are obtained.

An object, such as a molecule or nanoparticle, is chiral if it does not contain any plane of symmetry. In other words, its mirror image cannot be superimposed onto it. For optically active chiral molecules and nanoparticles, the absorption of light is different for left and right circularly polarized light (LCP and RCP, respectively). Indeed, circular dichroism (CD) refers to the difference in their absorption $\Delta\varepsilon \equiv \varepsilon_L - \varepsilon_R$, which is wavelength dependent. By sending equal amounts of LCP and RCP light to a sample and recording $\Delta\varepsilon$ at different wavelengths a unique, particle-dependent CD spectrum is obtained.

In the infrared region, CD spectroscopy can be used for structural studies of small organic molecules, proteins and DNA. The ability to measure CD spectra at red wavelengths is expected to refine such structural studies. In addition, chiral structures can lead to interesting optical effects such as superchiral electromagnetic fields. More generally, chirality is a fundamental asymmetry found in nature and it should be possible to use it for the design of artificial optical surfaces and colloids.

In this collaboration between researchers at DIPC and in Switzerland, Germany and South Korea, it is demonstrated that off-cut silicon wafers can provide a versatile approach to fabricate high-quality chiral surfaces as well as chiral colloidal nanoparticles with complex shapes difficult to obtain otherwise. The nanoparticles contain tips and binding pockets for exploration of enhanced detection of structural chirality. The obtained chiral colloids made from solid particles open possibilities in nonlinear optics, opto-fluidics, and photocatalysis.

We demonstrate that off-cut silicon wafers can provide a versatile approach to fabricate high-quality chiral surfaces as well as chiral colloidal nanoparticles with complex shapes




(a) Electron micrographs demonstrating the fabrication of chiral surfaces: (a1) Kite-shaped opening in a SiNx mask exposing a portion of a [137]-oriented Si wafer. The in-plane orientation of the Si is shown. (a2) Experimental etch pit from anisotropic etching of (a1). (a3) Simulated etch pit for the experimental structure in (a1). (a4) A series of experimental etch pits obtained by rotating the kite-shaped opening in (a1). Starting at the bottom left, the kite is rotated in 5° steps counterclockwise for each pit moving up each column and then left to right. The top left pit is (a2). (a5) Array of chiral pyramids obtained by depositing 400 nm of Au on (d) followed by template stripping.

(b) Electron micrographs demonstrating the fabrication of chiral colloids: (b1) Left-handed etch pit formed by anisotropic etching of Si{137}, observed through a circular 425 nm opening in a SiNx mask. (b2) 50 nm of Au deposited in the etch pit in (b1). Au deposited on the horizontal portions of the mask was previously removed via Scotch tape. (b3) Left-handed Au nanoparticle (415 nm base diameter) extracted from an etch pit as in (b1). The nanoparticle rests on an underlying Ag film deposited after Au. Inset: Simulated side view of the expected chiral shape of the nanoparticle. (b4-b5) Array of left/right-handed Au nanoparticles extracted from an array of etch pits as in (b1) on Si{137}/Si{$\bar{1}\bar{3}\bar{7}$} (200/190 nm base diameter, respectively). The nanoparticles rest on a Ag film. (b6-b7) Optical photographs of 2 mL of a 10 pM dispersion in dimethylformamide (DMF) of left-handed Au nanoparticles (as in b7) in reflection and transmission, respectively. (b8) A dense film of the left-handed Au nanoparticles dried from a dispersion on a substrate. (b9) Experimental circular dichroism (CD) signals in millidegrees of ellipticity versus wavelength for Au nanoparticles. Blue/red line corresponds to left/right-handed particles (200 nm base diameter) measured for 1 mm path length of a 1 pM dispersion in DMF.

DIPC HIGHLIGHT 2014

# Coherent ultrafast charge transfer in an organic photovoltaic blend

S. Maria Falke, C.A. Rozzi, D. Brida, M. Amato, A. De Sio, A. Rubio, G. Cerullo, E. Molinari and C. Lienau
*Science 344*, 6187 (2014)

**Silicon panel-based technology requires a very costly, contaminating manufacturing process, while organic photovoltaic (OPV) devices have been positioned as one of the most attractive alternatives as a source of solar energy.**

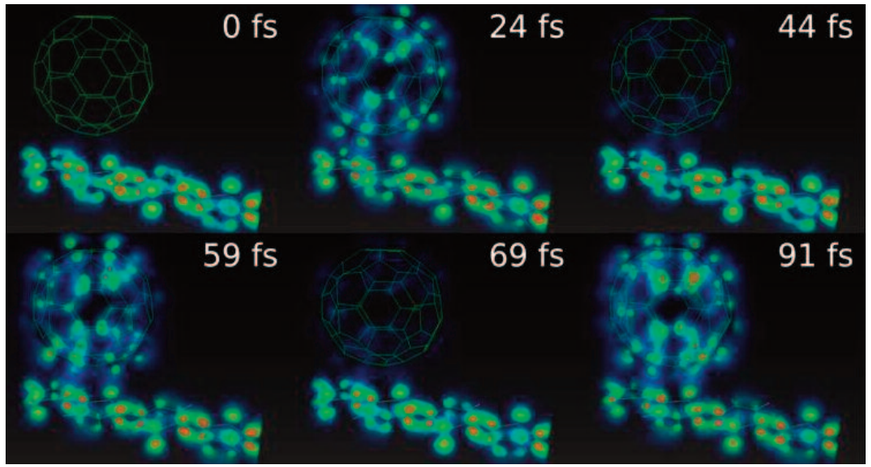
**This research has made a ground-breaking discovery** because it is the first time that the quantum mechanisms that trigger the photovoltaic function of these devices have been deciphered. Angel Rubio, Professor of Condensed Matter Physics at the Faculty of Chemistry of the UPV/EHU-University of the Basque Country, director of the Nano-Bio Spectroscopy Group, and associate researcher of the Donostia International Physics Center (DIPC), has participated in the research conducted in this field in collaboration with various centres in Germany, Italy and France. The research has been published in the prestigious journal Science.

These organic devices use a photosensitive polymer linked to a carbon nanostructure that functions as a current collector. When light falls on the device, the polymer traps the particles of light and induces the ultrafast transmission of electrons to the nanostructure through an electron impulse in the order of femtoseconds (fs), in other words, 10-15 seconds. Evidence was recently found to confirm this ultrafast transfer, but the research of Rubio and his team has gone a step further because it has succeeded in deciphering the elemental mechanism that unleashes the electron transfer between the polymer and the nanostructure. First principle theoretical simulations in a simplified model predicted that the coherent vibrations are the ones that dictate the periodic transfer of charge between the polymer and the fullerene.

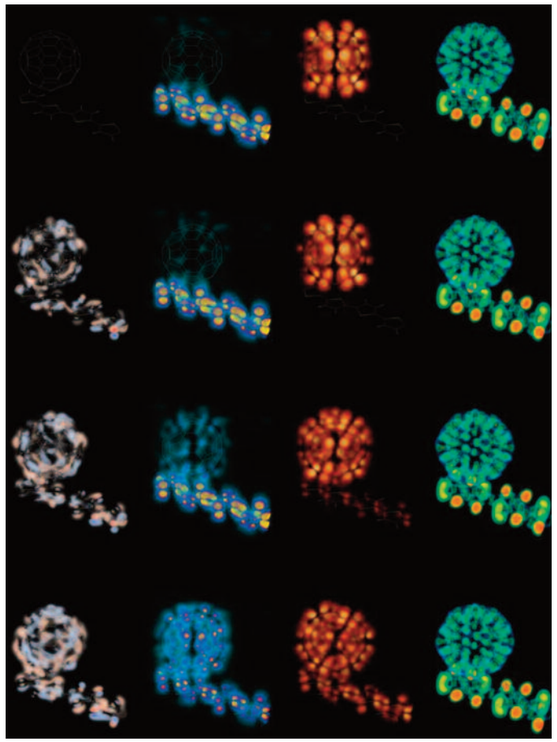
The experimental group confirmed this prediction by studying the optical response of a common material comprising a polymer and a by-product of the fullerene (a conventional nanostructure with a spherical shape) by means of high-resolution temporal spectroscopy.

The results confirmed that the coupling of the vibrations of the polymer and the fullerene bring about the electron transfer in a coherent and ultrafast way (≈23 fs), difficult to reconcile with incoherent processes that are manifested in slower transfers (100 fs). These studies demonstrate the critical role played by quantum coherence in organic photovoltaic devices.

The research, offers a vision that is consistent with elemental quantum processes in organic photovoltaic devices and constitutes a significant step forward in this field.



Photos of the simulation of the evolution in the transfer of charge from the polymer to the fullerene in femtoseconds.


Bottom to down: time evolution of the transfer of charge from the polymer after light exctiation to the fullerene in the time scale of femtoseconds projected on the orbitals (HOMO and LUMO) of the fullerene and polymer.

The quantum mechanisms of organic devices for alternative solar panels are revealed

# Anisotropic dispersion and partial localization of acoustic surface plasmons on an atomically stepped surface: Au(788)

M. Smerieri, L. Vattuone, L. Savio, T. Langer, C. Tegenkamp, H. Pfnür, V. M. Silkin, and M. Rocca
*Physical Review Letters 113*, 186804 (2014)

**Understanding acoustic surface plasmons (ASPs) in the presence of nanosized gratings is necessary for the development of future devices that couple light with ASPs. We show here by experiment and theory that two ASPs exist on Au(788), a vicinal surface with an ordered array of monoatomic steps. The ASPs propagate across the steps as long as their wavelength exceeds the terrace width, thereafter becoming localized. Our investigation identifies, for the first time, ASPs coupled with intersubband transitions involving multiple surface-state subbands.**

**Acoustic Surface Plasmons (ASP) originate from** the excitation of a two-dimensional (2D) electron gas whenever it is effectively screened by an underlying 3D electron gas as, eg, it occurs at the noble-metal surfaces. Contrary to sheet plasmons, characterized by a square-root like dependence on wavevector, ASPs have a linear soundlike dispersion and hence a frequency-independent group and phase velocities. These excitations are very promising for future applications in plasmonics since the speed and thus the wavelength of ASPs is three orders of magnitude lower than that of light, permitting us in principle to locate plasmonic excitations on the scale of a few nanometers. A hypothetical polychromatic ASP signal would indeed propagate without distortion, allowing for accurate signal processing.

The dispersion curves of ASP and light do, however, per se not cross at clean surfaces so a momentum source is needed to realize coupling of the ASP with photons; this can be realized by, eg, a grating. However, the short wavelength of the ASP requires realization of this grating on the atomic scale. Nano-structuring, however, implies concomitant generation of atomic defects, so it is necessary to understand how defects and confinement in nanosized regions modify the ASP dispersion. Combining the energy loss spectroscopy - low energy electron diffraction (ELS-LEED) experiment and density-response calculations, we demonstrate here the existence of two plasmonic modes at the Au(788) surface both parallel and perpendicular to the steps, due to the splitting of the Shockley surface state (SSS) band existing of the bare Au(111) surface into separate subbands caused by the step potential as shown in Figure 1.

The measured plasmon peak positions are collected in Figure 2. Our data clearly indicate that two losses with sound-like dispersion are present, denoted by I and II in Figure 2a). Across the steps the data points level out at large $q_{||}$. The branch with the steeper slope originates clearly from the ASP associated to the SSS of the (111) terraces, which has a very similar slope as on flat Au(111), while the lower branches have no counterpart on pristine Au(111).



These findings lead to the following remarkable physical scenario:
(a) Along the steps we observe two ASP modes with different group velocities determined by the maximal Fermi velocities of two partly occupied SSS subbands.
(b) The anisotropy introduced by the steps on Au(788) does not automatically lead to plasmon localization normal to the terraces, but the SSS subband formation is reflected by a splitting of the ASP also normal to the steps.
(c) The QW1 and QW2 subbands are still able to generate propagating plasmonic modes across the steps at wavelengths longer than the terrace width. The slightly different slopes of the modes parallel and normal to the steps reflect the anisotropy of the system.
(d) Across the steps signs of plasmon localization become visible when $q_{||}$ exceeds the reciprocal lattice vector $G_0$ of the periodic step array, and get more and more dominant when multiples of $G_0$ can be transferred. Together with an increasing efficiency of momentum transfer at steps with decreasing plasmon wavelength this leads to nearly complete localization at the highest $q_{||}$ of present measurements.

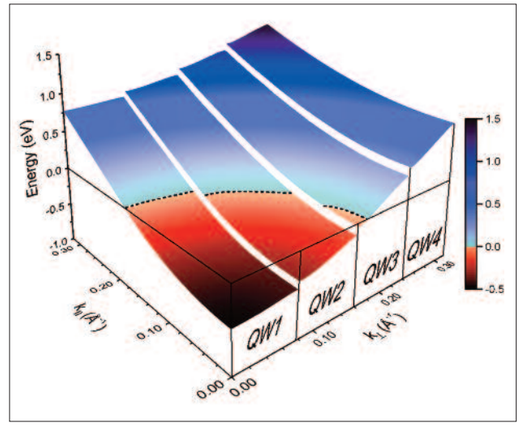



Figure 1. Surface-state dispersion in the extended band scheme for Au(788) calculated for the 1D model and used to fit the photoemission data. The dotted lines show the Fermi level in each quantum-well subband.

A mechanism of acoustic surface plasmon localization by atomic steps is uncovered on Au(788) vicinal surface.

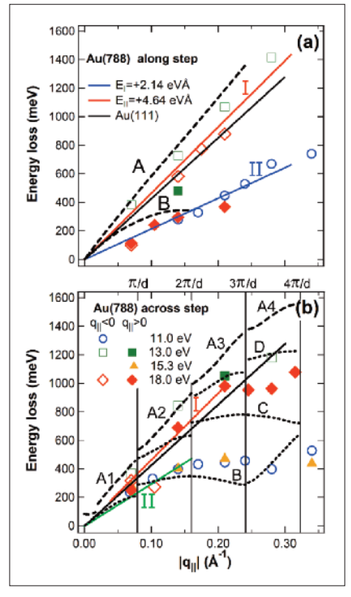



Figure 2. EEL peak positions, as measured at room temperature by ELS-LEED on Au(788) (a) along and (b) across the steps, vs. exchanged in-plane momentum $q_{||}$ and comparison with theory. The red lines correspond to the linear best fit to the isotropic higher-energy branch. Blue and green lines are a similar fit for the lower-energy branch along and across the steps, respectively, where across the steps the fit was limited to $q_{||} < 0.16$ Å$^{-1}$. Open and filled symbols correspond to experimental data collected, respectively, at positive and negative $q_{||}$. The solid black line is the dispersion of the ASP at the bare Au(111) surface. Dashed and dotted lines indicate the theoretical plasmon modes dispersion.

# Superconductor-ferromagnetic insulator structures for thermoelectric devices

F.S. Bergeret, F. Giazotto, T.T. Heikkilä, J.S. Moodera, A. Ozaeta, J.W.A. Robinson and P. Virtanen
*Physical Review Letters 112*, 057001 (2014) and *Applied Physics Letters 105*, 062602 (2014)

**Large thermoelectric power from a combination of magnets and superconductors thermoelectric devices can cool materials by passing currents, or convert temperature differences into electric power. However, especially metallic structures have a very poor thermoelectric performance, and therefore most thermoelectric are made of semiconductors.**

**Last year Asier Ozaeta and F. Sebastian Bergeret** from the Mesoscopic Physics Group at DIPC (Donostia-San Sebastian) in collaboration with researchers from the University of Jyväskylä and Aalto University (Finland), have shown how a proper combination of magnetic metals and superconductors could allow reaching very high thermoelectric conversion efficiency. The electronic structure of semiconductors and superconductors looks superficially similar, because both contain an "energy gap", a region of energies forbidden for the electrons. The difference between the two is that doping semiconductors allows moving this energy gap with respect to the average electron energy. This is in contrast to superconductors, where the energy gap is symmetric with respect to positive and negative energies, and therefore the thermoelectric effect from positive energy electrons cancels the effect from the negative energy electrons. In the first work published in 2014, Ozaeta, Bergeret and the international research group showed how this symmetry can be broken within the superconductor with a spin-split density of states induced by the proximity of a ferromagnetic insulator (Figure 1). As a result, the system exhibits a very large thermoelectric effect. Because conventional superconductors require temperatures of the order of a few Kelvin, this mechanism cannot be used directly in consumer devices such as portable coolers or waste heat converters. However, it could be used in accurate signal detection, or a similar mechanism could be applied in semiconductors to improve their thermoelectric performance.

In a subsequent work, F. Sebastián Bergeret in collaboration with reasearchers from the Scoula Normale Superiore in Pisa (Italy), Cambridge University (UK) and the Massachusetts Institute of Technology (USA), demonstrated that the efficiency of such devices can be considerably improved if the superconductor-ferromagnetic insulator element is embedded in a superconducting loop. In such a case a very large Seebeck coefficient of the order of mV/K can be achieved, leading to a figure-of-merit (ZT) far exceeding the values of state-of-the-art thermoelectric materials (Figure 2).

One of the published works was chosen as an "Editor's suggestion" category in *Physical Review Letters*, recommending articles for wide range of people because of their clarity.

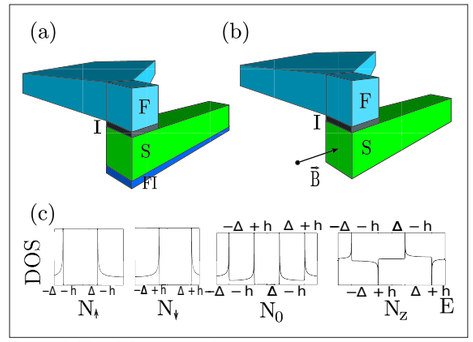



Figure 1. The S-FI thermoelectric element.
(a) Schematic representation of the superconductor (S) ferromagnetic insulator (FI) with a ferromagnetic (F) injector; (b) realization of the thermoelectric element by applying an external field. (c) Spin-split of the density of states of the superconductor that leads to the large thermoelectric effect.

The performance of S-FI thermoelectric devices can be much larger that the hitherto known thermoelectric materials.

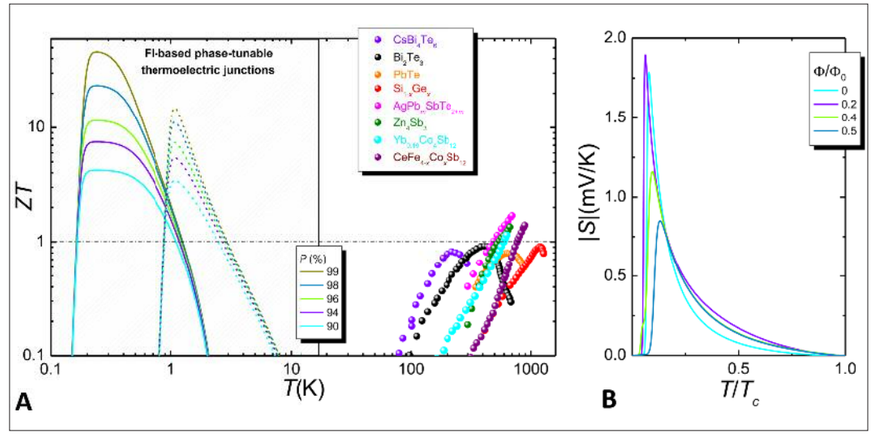



Figure 2. Thermoelectric efficiency of the thermoelectric element embedded in a superconducting loop. Comparison of the S-FI transistor performance with state-of-the-art high-ZT materials and the achievable Seebeck coefficient. (a) Left side: Expected figure of merit ZT vs T for an EuS/Al-type (solid lines) and GdN/NbN-type (dashed lines) phase-coherent thermoelectric transistors calculated for selected values of the barrier polarization. Right side: Figure of merit ZT vs temperature possessed by several state-of-the-art commercial bulk thermoelectric materials. Dash-dotted line indicates ZT=1. (b) Absolute value of the Seebeck coefficient (S) achievable in the S-FI thermoelectric transistor vs T calculated for a few selected values of the applied magnetic flux through the superconducting loop.

# Threading plasmonic nanoparticle strings with light

L.O. Herrmann, V.K. Valev, C. Tserkezis, J.S. Barnard, S. Kasera, O.A. Scherman, J. Aizpurua and J.J. Baumberg
*Nature Communications 5*, 4568 (2014)

**A new technique which uses light like a needle to thread long chains of metallic particles allows to modify their optical response and could help bring novel material concepts such as cloaking devices one step closer to reality.**

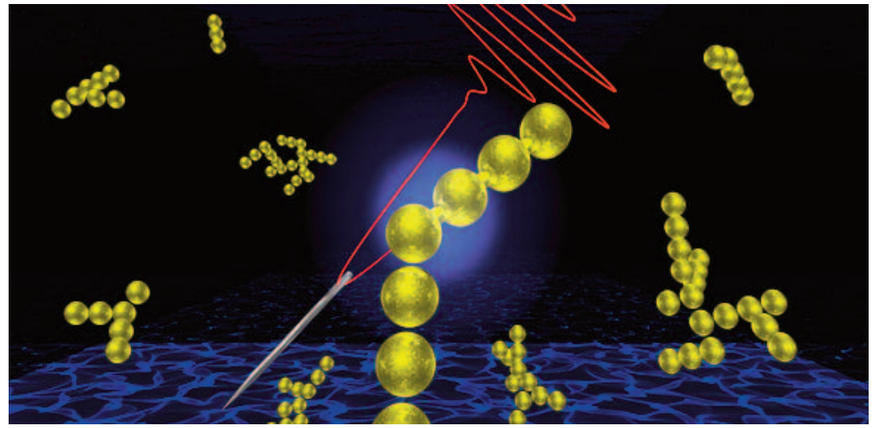
**A new method of building and manipulating materials** using light, developed and analyzed by researchers at the University of Cambridge (UK) and Donostia International Physics Center (DIPC), could one day enable technologies that are often considered the realm of science fiction, such as invisibility cloaks and cloaking devices. Although cloaked starships won't be a reality for quite some time, the technique which researchers have developed for constructing materials with building blocks a few billionths of a metre across can be used to control the way that light flies through them, and works on large chunks all at once. Details are published in the journal Nature Communications.

The technique developed by the Cambridge team involves using unfocused laser light as billions of electromagnetic needles, literally stitching gold nanoparticles together into long strings, directly in water for the first time. These strings can then be stacked into layers one on top of the other, similar to Lego bricks. The method makes it possible to produce materials in much higher quantities than can be made through current techniques. These nanoparticle strings show clear resonances in their response to light that can be tuned from the visible to the infrared, and might constitute the building blocks of novel metamaterials that show technologically relevant properties such as negative refraction index or broadband cloaking materials.

In order to make the strings, the researchers first used barrel-shaped molecules called cucurbiturils (CBs). The CBs act like miniature spacers, enabling a very high degree of control over the spacing between the nanoparticles, locking them in place. In order to connect them electrically, the researchers needed to build a bridge between the nanoparticles. Conventional welding techniques would not be effective, as they cause the particles to melt. The challenging aspect of this novel synthesis is to precisely control the bridge between nanoparticles as well as scaling up the process of particle linking. The key to controlling the bridges lies in the cucurbiturils: the precise spacing between the nanoparticles allows much more control over the process. When the laser is focused on the strings of particles in their CB scaffolds, it produces plasmons: ripples of electrons at the surfaces of conducting metals. These skipping electrons concentrate the light energy on atoms at the surface and join them to form bridges between the nanoparticles, acting as effective electromagnetic needles that physically sew these nanoblocks. Using ultrafast lasers results in billions of these bridges forming in rapid succession, threading the nanoparticles into long strings, which can be monitored in real time.

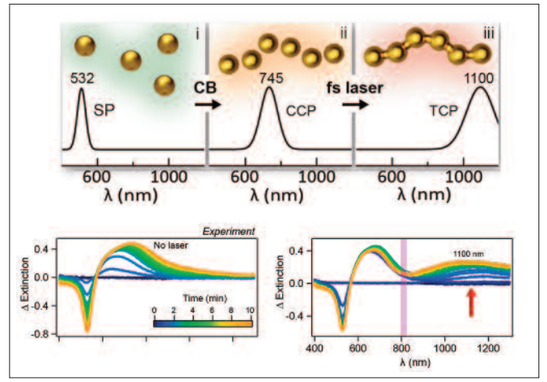
The active formation of strings of particles is unambiguously identified thanks to a peculiar optical fingerprint that characterizes "linked" particles: a mid-infrared plasmonic peak emerges in the optical spectrum as the threaded nanoparticles are formed, and both the position and width of this novel peak are tremendously sensitive to the geometrical details of the interparticle bridge formed. An excellent agreement between the optical fingerprints of the bridges experimentally created in Cambridge and those of the model bridges simulated at DIPC helps to understand the dynamics and morphology of the nanoparticle-string creation.

Dr. Ventsislav Valev, the leading researcher within the team of Prof. J.J. Baumberg in Cambridge worked with researchers from the Department of Chemistry, the Department of Materials Science & Metallurgy, and researchers of the "Theory of Nanophotonics Group" at the Donostia International Physics Center on the project.



Schematics of metallic nanoparticles being threaded by a light pulse. Light is concentrated in between the particles producing a physical link that unites them in long chains.

## 'Invisible' materials can be built by threading with light




(Top) Schematics of the evolution of the spectral response of nanoparticle chains showing the evolution of their plasmonic resonances. Left: resonance of isolated nanoparticles. Middle: resonance of an aggregate of nanoparticles. Right: resonance of a thread of nanoparticles glued by light. (Bottom) Left: Experimental spectroscopy showing the evolution of the plasmonic resonance as the nanoparticles aggegate. Right: Evolution of the plasmonic resonance as the particles are threaded by light.

DIPC HIGHLIGHT 2014

# Aromaticity in transition structures

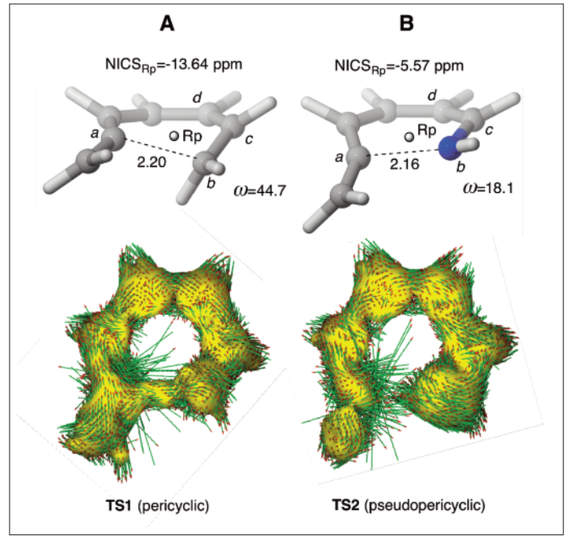
P. v. Ragué Schleyer, J. I. Wu, F. P. Cossío and I. Fernández
*Chemical Society Reviews 43,* 4909-4921 (2014)

**Aromaticity is an essential concept in chemistry and physics, employed to account for the unusual stability, reactivity, molecular structures, and other properties of many unsaturated organic compounds. This concept was later extended to systems with mobile electrons, as well as to transition structures. Although transition structures are inherently delocalized, not all exhibit aromaticity. We contrast examples of pericyclic reaction transition structures (where aromaticity is significant) with those for illustrative pseudo- and non-pericyclic reactions.**

**In 2014 Dr. I. Fernández and DIPC researcher Prof. F. P. Cossío** were invited to coordinate as Editors a themed issue of Chemical Society Reviews (cf. I. Fernández, F. P. Cossío, Chem. Soc. Rev. 2014, 43, 4906-4908). The title of this issue was "Applied Computational Chemistry", in line with the concept of "Applied Theoretical Chemistry" coined by Prof. Roald Hoffmann. This themed issue was hence focused on the application of computational/ theoretical methods to problems of interest to a wide experimental audience.

This paper summarizes current computational methods for identifying aromatic transition structures, with special emphasis on magnetic criteria. It also illustrates representative examples of pericyclic, pseudo-pericyclic and non-pericyclic reactions involving aromaticity. In pericyclic transformation aromatic stabilization of the corresponding transition states is very important, whereas in pseudo- and non-pericyclic reactions aromaticity is less or not relevant. The tremendous development of computational chemistry during the past few decades provides chemists and physicists with a robust theoretical framework and very helpful tools to generalize the concept of aromaticity and its application to transition structures, which are not accessible for a direct experimental study. The computation-based discovery that aromatic transition states can participate in non-pericyclic reactions exemplifies the effectiveness of theoretical approaches for recognizing novel chemical transformations. Despite caveats that aromaticity is just a chemical bonding model without a quantifiable, precise meaning, it remains a highly popular and essential concept in chemistry and physics accounting for anomalous properties such as geometry, reactivity and magnetic behaviour. A detailed analysis of aromaticity in transition structures extends the applicability of this concept to "closed circuit" structures involved in the transformation of matter via cyclic molecular mechanisms.

Unfortunately this paper is the coda to the collaboration between one research team of DIPC and late Professor Paul von Ragué Scheleyer, who passed away on Nov. 21, 2014 (cf. Henry F. Schaefer, Nature, 2015, 517, 22; G. A. Olah and G. K. Surya Prakash, Angewandte Chemie Int. Ed., 2015, 54, 2322-2323).




Two examples of pericyclic aromatic (A) and pseudopericyclic non-aromatic (B) transition structures. Diagrams shown below represent electron density and electronic circulation in the presence of a magnetic field.

Applied Computational Chemistry focuses on the application of theoretical methods to problems of interest to a wide experimental audience.


Cover of the ChemSocRev themed issue on "Applied Computational Chemistry". Invited Editors: I. Fernández and F. P. Cossío.

# Strong ferromagnetism at the surface of an antiferromagnet caused by buried magnetic moments

A. Chikina, M. Hoppner, S. Seiro, K. Kummer, S. Danzenbacher, S. Patil, A. Generalov, M. Guttler, Yu. Kucherenko, E.V. Chulkov, Yu. M. Koroteev, K. Kopernik, C. Geibel, M. Shi, M. Radovic, C. Laubschat, and D.V. Vyalikh

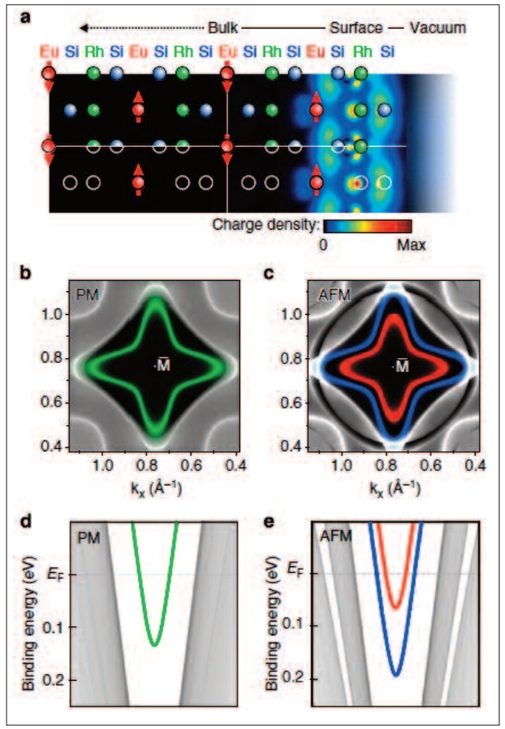
*Nature Communications 5*, 3171 (2014)

**Here we show that the Si-Rh-Si surface trilayer of the antiferromagnet $EuRh_2Si_2$ bears a surface state, which exhibits an unexpected and large spin splitting controllable by temperature. The splitting sets in below 32.5 K, well above the ordering temperature of the Eu 4*f* moments (24.5 K) in the bulk, indicating a larger ordering temperature in the topmost Eu layers. The driving force for the itinerant ferromagnetism at the surface is the aforementioned exchange interaction. Such a splitting may also be induced into states of functional surface layers deposited onto the surface of $EuRh_2Si_2$ or similarly ordered magnetic materials with metallic or semiconducting properties.**

**For a long time, rare-earth intermetallic materials** have attracted considerable interest because of their exotic properties at low temperatures, which include complex magnetic phases, valence fluctuations, heavy-fermion states, Kondo behaviour and many others. $EuRh_2Si_2$ is apparently well-suited to give insight into the interplay between magnetic and electronic degrees of freedom. Its electronic structure is strongly correlated, involving massless and heavy quasiparticles, which are mutually interacting. Below the Neel temperature 24.5K the Eu 4*f* moments in $EuRh_2Si_2$ order antiferromagnetically (AFM). Like in several other $RERh_2Si_2$ compounds, the magnetic structure of $EuRh_2Si_2$ is composed of ferromagnetic Eu layers in the ab planes stacking AFM along the c axis.

Here we report on strong ferromagnetic properties of the surface and subsurface region in the antiferromagnet $EuRh_2Si_2$, which are driven by the ordered local 4*f* moments of Eu. These properties are monitored by angle-resolved photoelectron spectroscopy and density functional theory calculations looking at the diamond-shaped surface state that exists around the M point of the surface Brillouin zone. This Shockley-type surface state is observed at the Si-terminated surface, and resides inside a large gap in the projected bulk band structure. The surface ferromagnetism is manifested by a huge splitting of this state due to the exchange interaction with the ordered local moments of the Eu atoms lying three atomic layers below the surface. The exchange splitting of the surface state, which may be described as a trapped two-dimensional electron gas within the top four layers, provides immediate information on the magnetism of the first buried Eu layer in $EuRh_2Si_2$ when followed, for instance, as a function of temperature.

In summary, we have given clear evidence for a large exchange coupling of a Si-derived Shockley surface state to the outermost Eu layer that is located four atomic layers below the surface of the antiferromagnetic compound $EuRh_2Si_2$. The resulting exchange splitting provides direct information on the temperature dependent magnetism in the Eu layer and reveals an ordering temperature of 4*f* moments close to the surface that is notably higher than the bulk TN. Our results suggest that the mechanism of formation of the surface ferromagnetism discovered in $EuRh_2Si_2$ can be extended to other antiferromagnetic metallic or semiconducting compounds where surface states exist in an energy gap at the Fermi level. These spin-split surface states may induce magnetization in functional surface layers of topological insulators or/and Rashba-type surface systems deposited onto the antiferromagnetic material, thus opening an energy gap in the topological or Rashba-type surface states.




(a) Probability density distribution (projected on the ac plane) of the surface states at the M point obtained for the paramagnetic (PM) phase, which is superimposed with the slab crystal structure used for band-structure calculations. (b,c) The computed and superimposed Fermi surfaces for bulk and slab calculations for the PM and AFM phases, respectively. Here, the diamond-shaped surface states lie in the huge gap (black) of the projected bulk bands (grey) around the M point. For the PM and AFM phases the surface state is shown in green (unsplit) and red-blue (split) colours, respectively. (d,e) Computed electron band structures along the line used in the experimental study of the temperature evolution of the surface state spin split.

The mechanism of formation of the surface ferromagnetism discovered in $EuRh_2Si_2$ can be extended to other antiferromagnetic metallic or semiconducting compounds.

# Publications

1 Chain dynamics on crossing the glass transition: nonequilibrium effects and recovery of the temperature dependence of the structural relaxation.
Arrese-Igor S, Alegria A, and Colmenero J.
ACS Macro Letters 3, 1215 (2014).

2 Cluster glasses of semiflexible ring polymer.
Slimani MZ, Bacova P, Bernabei M, Narros A, Likos CN, and Moreno AJ.
ACS Macro Letters 3, 611 (2014).

3 How far are single-chain polymer nanoparticles in solution from the globular state?
Pomposo JA, Perez-Baena I, Lo Verso F, Moreno AJ, Arbe A, and Colmenero J.
ACS Macro Letters 3, 767 (2014).

4 Metallo-folded single-chain nanoparticles with catalytic selectivity.
Sanchez-Sanchez A, Arbe A, Colmenero J, and Pomposo JA.
ACS Macroletters 3, 439 (2014).

5 Epitaxially connected PbSe quantum-dot films: controlled neck formation and optoelectronic properties.
Sandeep CSS, Azpiroz JM, Evers WH, Boehme SC, Moreels I, Kinge S, Siebbeles LDA, Infante I, and Houtepen AJ.
ACS Nano 8, 11499 (2014).

6 Spectroscopic fingerprints of work-function-controlled phthalocyanine charging on metal surfaces.
Borghetti P, Ei-Sayed A, Goiri E, Rogero C, Lobo-Checa J, Floreano L, Ortega JE, and de Oteyza DG.
ACS Nano 8, 12786 (2014).

7 Revealing the adsorption mechanisms of nitroxides on ultrapure, metallicity-sorted carbon nanotubes.
Ruiz-Soria G, Paz AP, Sauer M, Mowbray DJ, Lacovig P, Dalmiglio M, Lizzit S, Yanagi K, Rubio A, Goldoni A, Ayala P, and Pichler T.
ACS Nano 8, 1375 (2014).

8 Electrochemical control over photoinduced electron transfer and trapping in CdSe-CdTe quantum-dot solids.
Boehme SC, Walvis TA, Infante I, Grozema FC, Vanmaekelbergh D, Siebbeles LDA, and Houtepen AJ.
ACS NANO 8, 7067 (2014).

9 Luminescence, patterned metallic regions, and photon-mediated electronic changes in single-sided fluorinated graphene sheets.
Walter AL, Sahin H, Jeon KJ, Bostwick A, Horzum S, Koch R, Speck F, Ostler M, Nagel P, Merz M,Schupler S, Moreschini L, Chang YJ, Seyller T, Peeters FM, Horn K, and Rotenberg E.
ACS NANO 8, 7801 (2014).

10 Lasing threshold of one- and two-photon-pumped dye-doped silica powder.
Garcia-Ramiro B, Illarramendi MA, Garcia-Revilla S, Balda R, Levy D, Zayat M, and Fernandez J.
Applied Physics B-Lasers and Optics 117, 1135 (2014).

11 Photo-induced strengthening of weak bonding in noble gas dimers.
Miyamoto Y, Miyazaki T, Rubio A, and Zhang H.
Applied Physics Letters 104, 201107 (2014).

12 Modeling anisotropic plasmon excitations in self-assembled fullerenes.
Iurov A, Gumbs G, Gao B, and Huang D.
Applied Physics Letters 104, 203103 (2014).

13 Proposal for a phase-coherent thermoelectric transistor.
Giazotto F, Robinson JWA, Moodera JS, and Bergeret FS.
Applied Physics Letters 105, 062602 (2014).

14 Proximity nanovalve with large phase-tunable thermal conductance.
Strambini E, Bergeret FS, and Giazotto F.
Applied Physics Letters 105, 082601 (2014).

15 VLTI/AMBER observations of cold giant stars: atmospheric structures and fundamental parameters.
Arroyo-Torres B, Marti-Vidal I, Marcaide JM, Wittkowski M, Guirado JC, Hauschildt PH, Quirrenbach A, and Fabregat J.
Astronomy and Astrophysics 566, A88 (2014).

16 Constraints on the progenitor system and the environs of SN 2014J from deep radio observations.
Perez-Torres MA, Lundqvist P, Beswick RJ, Bjornsson CI, Muxlow TWB, Paragi Z, Ryder S, Alberdi A, Fransson C, Marcaide JM, Marti-Vidal I, Ros E, Argo MK, and Guirado JC.
Astrophysical Journal 792, 38 (2014).

17 Spectral and morphological analysis of the remnant of supernova 1987 a with alma and atca.
Zanardo G, Staveley-Smith L, Indebetouw R, Chevalier RA, Matsuura M, Gaensler BM, Barlow MJ, Fransson C, Manchester RN, Baes M, Mamenetzky JR, Lakicevic M, Lundqvist P, Marcaide JM, Marti-Vidal I, Meixne M, Ng CY, Park S, Sonneborn G, Spyromilio J, and van Loon JT.
Astrophysical Journal 796, 82 (2014).

18 Could the lithium bond be classified as the r-hole bond? – QTAIM and NBO analysis.
Lipkowski P, and Grabowski SJ.
Chemical Physics Letters 591, 113 (2014).

19 Halogen bond with the multivalent halogen acting as the Lewis acid center.
Grabowski, SJ.
Chemical Physics Letters 605, 131 (2014)

20 Adsorption of tetrathiafulvalene (TTF) on Cu(100): can pi-stacked 1-D aggregates be formed at low temperature?
Sarasola A, Barja S, de Parga ALV, and Arnau A.
Chemical Physics Letters 612, 45 (2014)

21 Applied computational chemistry.
Fernandez I, and Cossio FP.
Chemical Society Reviews 43, 4906 (2014).

22 Aromaticity in transition structures.
Schleyer PV, Wu JI, Cossio FP, and Fernandez I.
Chemical Society Reviews 43, 4909 (2014).

23 DNA intercalating Ru-II polypyridyl complexes as effective photosensitizers in photodynamic therapy.
Mari C, Pierroz V, Rubbiani R, Patra M, Hess J, Spingler B, Oehninger L, Schur J, Ott I, Salassa L, Ferrari S, and Gasser G.
Chemistry-A European Journal 20, 14421 (2014).

24 Distortions of pi-coordinated arenes with anionic character.
Falceto A, Casanova D, Alemany P, and Alvarez S.
Chemistry-A European Journal 20, 14674 (2014).

25 Cytotoxic gold(I) N-heterocyclic carbene complexes with phosphane ligands as potent enzyme inhibitors.
Rubbian R, Salassa L, de Almeida A, Casini A, and Ott I.
Chemmedchem 9, 1205 (2014).

26 Boron and other triel Lewis acid centers: from hypovalency to hypervalency.
Grabowski SJ.
Chemphyschem: a European journal of chemical physics and physical chemistry 15, 2985 (2014).

27 Clusters of ammonium cation-hydrogen Bond versus sigma-hole Bond.
Grabowski SJ.
Chemphyschem: a European journal of chemical physics and physical chemistry 15, 876 (2014).

28 Coverage dependence of the level alignment for methanol on $TiO_2$(110).
Migani A, and Mowbray DJ.
Computational and Theoretical Chemistry 1040, 259 (2014).

29 New 'aggregation induced emission (AIE)' active cyclometalated iridium(III) based phosphorescent sensors: high sensitivity for mercury(II) ions.
Alam P, Kaur G, Climent C, Pasha S, Casanova D, Alemany P, Choudhury AR, and Laskar IR.
Dalton Transactions 43, 16431 (2014).

30 Contribution of evanescent waves to the effective medium of disordered waveguides.
Yepez M, and Saenz JJ.
EPL 108, 17006 (2014).

31 Structural and electronic properties of magnetic cylinders at the atomic scale.
Aguilera-Granja F, Montejano-Carrizales JM, and Vogel EE.
European Physical Journal D 68, 38 (2014).

32 High pressure phases of different tetraboranes.
Suarez-Alcubilla A, Gurtubay IG, and Bergara A.
High Pressure Research 34, 59 (2014).

33 Stereochemistry of complexes with double and triple metal-ligand bonds:
a continuous shape measures analysis.
Alvarez S, Menjon B, Falceto A, Casanova D, and Alemany P.
Inorganic Chemistry 53, 12151, (2014).

34 Application of the level set method for the visual representation of continuous
cellular automata oriented to anisotropic wet etching.
Montoliu C, Ferrando N, Cerdá J and Colom RJ.
International Journal of Computer Mathematics 91, 124 (2014).

35 Hole-phonon relaxation and photocatalytic properties of titanium dioxide and zinc oxide:
first-principles approach.
Zhukov VP, Tyuterev VG, Chulkov EV, and Echenique PM.
International Journal of Photoenergy 738921 (2014).

36 Perspective on natural orbital functional theory.
Piris M, and Ugalde JM.
International Journal of Quantum Chemistry 114, 1169 (2014).

37 Are there really Cooper pairs and persistent currents in aromatic molecules?
Squire RH, March NH, and Rubio A.
International Journal of Quantum Chemistry 114, 437 (2014).

38 Atomic structure and phonons of a Pb ultrathin film on the Al(100) surface.
Rusina GG, Borisova SD, and Chulkov EV.
Jetp Letters 100, 237 (2014).

39 Dynamics of the BiTeI lattice at high pressures.
Ponosov YS, Kuznetsova TV, Tereshchenko OE, Kokh KA, and Chulkov EV.
Jetp Letters 98, 557 (2014).

40 The phase equilibria in the $Ag_2S$-$Ag_8GeS_6$-$Ag_8SnS_6$ system.
Aliyeva ZM, Bagheri SM, Aliev ZS, Alverdiyev IJ, Yusibov YA, and Babanly MB.
Journal of Alloys and Compounds 611, 395 (2014).

41 Dielectric spectroscopy at the nanoscale by atomic force microscopy:
A simple model linking materials properties and experimental response.
Miccio LA, Kummali MM, Schwartz GA, Alegria A, and Colmenero J.
Journal of Applied Physics 115, 184305 (2014).

42 Local versus global electronic properties of chalcopyrite alloys:
X-ray absorption spectroscopy and ab initio calculations.
Sarmiento-Perez R, Botti S, Schnohr CS, Lauermann I, Rubio A, and Johnson B.
Journal of Applied Physics 116, 093703 (2014).

43 Dielectric spectra broadening as a signature for dipole-matrix interaction. IV.
Water in amino acids solutions.
Levy E, Cerveny S, Ermolina I, Puzenko A, and Feldman, Y.
Journal of Chemical Physics 140, 135104 (2014).

44 Second-order perturbative corrections to the restricted active space configuration
interaction with the hole and particle approach.
Casanova D.
Journal of Chemical Physics 140, 144111 (2014).

45 The interaction of organic adsorbate vibrations with substrate lattice waves in methyl-Si(111)-(1×1).
Brown RD, Hund ZM, Campi D, O'Leary LE, Lewis NS, Bernasconi M, Benedek G, and Sibener SJ.
Journal of Chemical Physics 141, 024702 (2014).

46 Interacting pairs in natural orbital functional theory.
Piris M.
Journal of Chemical Physics 141, 044107 (2014).

47 Ab initio molecular dynamics calculations on scattering of hyperthermal H atoms from
Cu(111) and Au(111).
Kroes GJ, Pavanello M, Blanco-Rey M, Alducin M, and Auerbach DJ.
Journal of Chemical Physics 141, 054705 (2014).

48 Quasi-particle energy spectra in local reduced density matrix functional theory.
Lathiotaki NN, Helbig N, Rubio A, and Gidopoulos NI.
Journal of Chemical Physics 141, 164120 (2014).

49 Two new constraints for the cumulant matrix.
Ramos-Cordoba E, Salvador P, Piris M, and Matito E.
Journal of Chemical Physics 141, 234101 (2014).

50 Vibrational lifetimes of hydrogen on lead films: An ab initio molecular dynamics with
electronic friction (AIMDEF) study.
Saalfrank P, Juaristi JI, Alducin M, Blanco-Rey M, and Diez Muino R.
Journal of Chemical Physics 141, 234702 (2014).

51 Nonadiabatic and time-resolved photoelectron spectroscopy for molecular systems.
Flick J, Appel H, and Rubio A.
Journal of Chemical Theory and Computation 10, 1665 (2014).

52 Quasiparticle level alignment for photocatalytic interfaces.
Migani A, Mowbray DJ, Zhao J, Petek H, and Rubio A.
Journal of Chemical Theory and Computation 10, 2103 (2014).

53 New approximation to the third-order density. Application to the calculation of correlated multicenter indices.
Feixas F, Sola M, Barroso JM, Ugalde JM, and Matito E.
Journal of Chemical Theory and Computation 10, 3055 (2014).

54 Electronic structure study of singlet fission in tetracene derivatives.
Casanova D.
Journal of Chemical Theory and Computation 10, 324 (2014).

55 Benchmark assessment of density functional methods on group II–VI MX (M = Zn, Cd; X = S, Se, Te) quantum dots.
Azpiroz JM, Ugalde JM and Infante I.
Journal of Chemical Theory and Computation 10, 76 (2014).

56 A survey of the parallel performance and accuracy of poisson solvers for electronic structure calculations.
Garcia-Risueño P, Alberdi-Rodriguez J, Oliveira MJT, Andrade X, Pippig M, Muguerza J, Arruabarrena A, and Rubio A.
Journal of Computational Chemistry 35, 427 (2014).

57 How much tetraradical character is present in the $Si_6$ $Ge_9$ cluster?
Casanova D.
Journal of computational chemistry 35, 944 (2014).

58 Electron dynamics of unoccupied states in topological insulators.
Niesner D, Otto S, Fauster T, Chulkov EV, Eremeev SV, Tereshchenko OE, and Kokh KA.
Journal of Electron Spectroscopy and Related Phenomena 195, 258 (2014).

59 Formation of metal-organic interface states studied with 2PPE.
Marks M, Scholl A, and Hofer U.
Journal of Electron Spectroscopy and Related Phenomena 195, 263 (2014).

60 Unoccupied electronic structure and relaxation dynamics of Pb/Si(111).
Sandhofe M, Sklyadneva IY, Sharma V, Trontl VM, Zhou P, Ligges M, Heid R, Bohnen KP, Chulkov EV,and Bovensiepen U.
Journal of Electron Spectroscopy and Related Phenomena 195, 278 (2014).

61 Whispering gallery mode emission from a composite system of J-aggregates and photonic microcavity.
Melnikau D, Savateeva D, Rusakov KI, and Rakovich YP.
Journal of Luminescence 145, 138 (2014).

62 Effect of $Tm^{3+}$ codoping on the near-infrared and upconversion emissions of $Er^{3+}$ in $TeO_2$-ZnO-$ZnF_2$ glasses.
Miguel A, Arriandiaga MA, Morea R, Fernandez J, Gonzalo J, and Balda R.
Journal of Luminescence 154, 136 (2014)

63 Structural, electronic and magnetic properties of ConPtM-n for M=13, 19, and 55, from first principles.
Montejano-Carrizales JM, Aguilera-Granja F, Goyhenex C, Pierron-Bohnes V, and Moran-Lopez, JL.
Journal of Magnetism and Magnetic Materials 355, 215 (2014).

64 Resistive switching dependence on atomic layer deposition parameters in $HfO_2$-based memory devices.
Zazpe R, Ungureanu M, Golmar F, Stoliar P, Llopis R, Casanova F, Pickup, DF, Rogero C, and Hueso LE.
Journal of Materials Chemistry C 2, 3204 (2014).

65 Anisotropic etching on Si{110}: experiment and simulation for the formation of microstructures with convex corners.
Pal P, Gosalvez MA, Sato K, Hida H, and Xing Y.
Journal of Micromechanics and Microengineering 24, 125001 (2014).

66 CdS nanoclusters doped with divalent atoms.
Jimenez-Izal E, Azpiroz JM, Gupta R, Matxain JM, and Ugalde JM.
Journal of Molecular Modeling 20, 2227 (2014).

67 Spin-orbit effects on the structural, homotop, and magnetic configurations of small pure and Fe-doped Pt clusters.
Alvarado-Leyva PG, Aguilera-Granja F, García-Fuente A, and Vega A.
Journal of Nanoparticle Research 16, 2222 (2014).

68 Carbo-cages: a computational study.
Azpiroz JM, Islas R, Moreno D, Fernandez-Herrera MA, Pan S, Chattaraj PK, Pratim K, Martinez-Guajardo G, Ugalde JM, and Merino G.
Journal of Organic Chemistry 79, 5463 (2014).

69 Linear and nonlinear optical effects induced by energy transfer from semiconductor nanoparticles to photosynthetic biological systems.
Rakovich A, Donegan JF, Oleinikov V, Molinari M, Sukhanova A, Nabiev I, and Rakovich YP.
Journal of Photochemistry and Photobiology C-Photochemistry Reviews 20, 17 (2014).

70 DFT/TDDFT study of the adsorption of N3 and N719 Dyes on ZnO(10(1)over-bar0) surfaces.
Azpiroz JM, and De Angelis F.
Journal of Physical Chemistry A 118, 5885 (2014).

71 Optical properties of 4-bromobenzaldehyde derivatives in chloroform solution.
Climent C, Alemany P, Lee D, Kim J, and Casanova D.
Journal of Physical Chemistry A 118, 6914 (2014).

72 Aluminum interaction with glutamate and alpha-Ketoglutarate: a computational study.
Mujika JI, Ugalde JM, and Lopez X.
Journal of Physical Chemistry B 118, 6680 (2014).

73 Evolutionary kinetic Monte Carlo: atomistic rates of surface-mediated processes from surface morphologies.
Ferrando, N, Gosalvez MA, and Ayuela A.
Journal of Physical Chemistry C 118, 11636 (2014).

74 Antiferromagnetism in Nanofilms of Mn-Doped GaN.
Echeverria-Arrondo C, Perez-Conde J, and Ayuela A.
Journal of Physical Chemistry C 118, 18064 (2014).

75 Asymmetric response toward molecular fluorination in binary Copper-Phthalocyanine/Pentacene assemblies.
de Oteyza DG. Garcia-Lastra JM, Goiri E, El-Sayed A, Wakayama Y, and Ortega, JE.
Journal of Physical Chemistry C 118, 18626 (2014).

76 Exploring the surface chemical reactivity of single crystals of binary and ternary bismuth chalcogenides.
Politano A, Caputo M, Nappini S, Bondino F, Magnano E, Aliev ZS, Babanly MB, Goldoni A, Chiarello G, and Chulkov EV.
Journal of Physical Chemistry C 118, 21517 (2014).

77 Identifying highly conducting Au-C links through inelastic electron tunneling spectroscopy.
Foti G, Vazquez H, Sanchez-Portal D, Arnau A, and Frederiksen T.
Journal of Physical Chemistry C 118, 27106 (2014).

78 Massive surface reshaping mediated by metal-organic complexes.
Abadia M, Gonzalez-Moreno R, Sarasola A, Otero-Irurueta G, Verdini A, Floreano L, Garcia-Lekue A, and Rogero C.
Journal of Physical Chemistry C 118, 29704 (2014).

79 Effect of structural dynamics on the opto-electronic properties of bare and hydrated ZnS QDs.
Azpiroz JM, Mosconi E, Ugalde JM, and De Angelis F.
Journal of Physical Chemistry C 118, 3274 (2014).

80 Quantum dot photoactivation of Pt(IV) Anticancer Agents: Evidence of an Electron Transfer mechanism driven by electronic coupling.
Infante I, Azpiroz JM, Blanco NG, Ruggiero E, Ugalde JM, Mareque-Rivas JC, and Salassa L.
Journal of Physical Chemistry C 118, 8712 (2014).

81 Resonant lifetime of core-excited organic adsorbates from first principles.
Fratesi G, Motta C, Trioni MI, Brivio GP, and Sanchez-Portal D.
Journal of Physical Chemistry C 118, 8775 (2014).

82 Natural orbital functional calculations of molecular polarizabilities and second hyperpolarizabilities. The hydrogen molecule as a test case.
Lopez X, Piris M, Nakano M, and Champagne B.
Journal of Physics B-atomic Molecular and Optical Physics 47, 015101 (2014).

83 Modelling the effect of nuclear motion on the attosecond time-resolved photoelectron spectra of ethylene.
Crawford-Uranga A, De Giovannini U, Mowbray DJ, Kurth S, and Rubio A.
Journal of Physics B-Atomic Molecular and Optical Physics 47, 124018 (2014).

84 Circular dichroism in XUV + IR multiphoton ionization of atoms.
Kazansky AK, Bozhevolnov AV, Sazhina IP, and Kabachnik NM.
Journal of Physics B: Atomic, Molecular and Optical Physics 47, 065602 (2014).

85 The origin of two-dimensional electron gases at oxide interfaces: insights from theory.
Bristowe NC, Ghosez P, Littlewood PB, and Artacho E.
Journal of Physics-Condensed Matter 26, 143201 (2014).

86 Electron-phonon coupling in quantum-well states of the Pb/Si(111) system.
Ligges M, Sandhofer M, Sklyadneva I, Heid R, Bohnen KP, Freutel S, Rettig L, Zhou P, Echenique PM, Chulkov EV, and Bovensiepen U.
Journal of Physics-Condensed Matter 26, 352001 (2014).

87 Species fractionation in atomic chains from mechanically stretched alloys.
da Silva Autreto PA, Galvao DS, and Artacho E.
Journal of Physics-Condensed Matter 26, 435304 (2014).

88 Structural characterization of slightly boron-deficient LiB, LiB0.9 and LiB0.8, under pressure.
Suarez-Alcubilla A, Gurtubay IG, and Bergara A.
Journal of Physics-Condensed Matter 26, 475402 (2014).

89 Use of surface plasmons for manipulation of organic molecule quasiparticles and optical properties.
Despoja V, and Marusic L.
Journal of Physics-Condensed Matter 26, 485012 (2014).

90 Structural modifications of gold thin films produced by thiol-derivatized single-stranded DNA immobilization.
Arroyo-Hernandez M, Svec M, Rogero C, Briones C, Martin-Gago JA, and Costa-Kramer JL.
Journal of Physics-Condensed Matter 26, 5, 055010 (2014).

91 Relaxation of highly excited carriers in wide-gap semiconductors.
Tyuterev VG, Zhukov VP, Echenique PM, and Chulkov EV.
Journal of Physics-Condensed Matter 27, 025801 (2014).

92 Anisotropic plasmon-coupling dimerization of a pair of spherical electron gases.
Gumbs G, Iurov A, Balassis A, and Huang D.
Journal of Physics-Condensed Matter: an Institute of Physics Journal 26, 135601 (2014).

93 Modelling near-surface bound electron states in a 3D topological insulator: analytical and numerical approaches.
Men'shov VN, Tugushev VV, Menshchikova V, Eremeev SV, Echenique PM, and Chulkov EV.
Journal of Physics. Condensed Matter: an Institute of Physics Journal 26, 485003 (2014).

94 Multiple scattering calculations for nonreciprocal planar magnetoplasmonic nanostructures.
Christofi A, Tserkezis C, and Stefanou N.
Journal of Quantitative Spectroscopy & Radiative Transfer 146, 34 (2014).

95 Differential capacitance of ionic liquid interface with graphite: the story of two double layers.
Kornyshev AA, Luque NB, and Schmickler, W.
Journal of Solid State Electrochemistry 18, 1345 (2014).

96 Photoinduced C-C reactions on insulators toward photolithography of graphene nanoarchitectures.
Palma CA, Diller K, Berger R, Welle A, Bjork J, Cabellos JL, Mowbray DJ, Papageorgiou AC, Ivleva NP, Matich S, Margapoti E, Niessner R, Menges B, Reichert J, Feng XL, Rader HJ, Klappenberger F, Rubio A, Mullen K, and Barth JV.
Journal of the American Chemical Society 136, 4651 (2014).

97 Structural, optical, and spectroscopic properties of $Er^{3+}$-doped $TeO_2$-ZnO-$ZnF_2$ glass-ceramics.
Miguel A, Morea R, Arriandiaga MA, Hernandez M, Ferrer FJ, Domingo C, Fernandez-Navarro JM, Gonzalo J, Fernandez J, and Balda R.
Journal of the European Ceramic Society 34, 3959 (2014).

98 The response of a $^3$He Fermi liquid droplet to vibronic excitation of an embedded glyoxal molecule.
Benedek G, Hizhnyakov V, and Toennies JP.
Journal Physical Chemistry A 118, 6574 (2014).

99 Time-resolved random laser spectroscopy of inhomogeneously broadened systems.
Fernandez J, Garcia-Revilla S, Carlos LD, Pecoraro E, Arriandiaga MA, and Balda R.
Laser & Photonics Reviews 8, L32 (2014).

100 Microscopic dynamics in nanocomposites of poly(ethylene oxide) and poly(methyl methacrylate) soft nanoparticles: a quasi-elastic neutron scattering study.
Bhowmik D, Pomposo JA, Juranyi F, Garcia-Sakai V, Zamponi M, Su Y, Arbe A, and Colmenero J.
Macromolecules 47, 1, 304 (2014).

101 Investigation of a nanocomposite of 75 wt % poly(methyl methacrylate) nanoparticles with 25 wt % poly(ethylene oxide) linear chains: a quasielatic neutron scattering, calorimetric, and WAXS study.
Bhowmik D, Pomposo JA, Juranyi F, Sakai VG, Zamponi M, Arbe A, and Colmenero J.
Macromolecules 47, 3005 (2014).

102 Branch-point motion in architecturally complex polymers: estimation of hopping parameters from computer simulations and experiments.
Bacova P, Lentzakis H, Read DJ, Moreno AJ, Vlassopoulos D, and Das Ch.
Macromolecules 47, 3362 (2014).

103 Collective features in polyisobutylene. A study of the static and dynamic structure factor by molecular dynamics simulations.
Khairy Y, Alvarez F, Arbe A, and Colmenero, J.
Macromolecules 47, 447 (2014).

104 Real-space analysis of branch point motion in architecturally complex polymers.
Bacová P. and Moreno AJ.
Macromolecules 47, 6955 (2014).

105 Efficient route to compact single-chain nanoparticles: photoactivated synthesis via thiol–yne coupling reaction.
Pérez-Baena I, Asenjo-Sanz I, Arbe A, Moreno AJ, Lo Verso F, Colmenero J, and Pomposo JA.
Macromolecules 47, 8270 (2014).

106 Intercalation and confinement of poly(ethylene oxide) in porous carbon nanoparticles with controlled morphologies.
Barroso-Bujans F, Palomino P, Fernandez-Alonso F, Rudic S, Alegria A, Colmenero J, and Enciso E.
Macromolecules 47, 8729 (2014).

107 Assessment of the second-order perturbative corrections to PNOF5.
Piris M, Ruiperez F, and Matxain JM.
Molecular Physics 112, 1 (2014).



108 Stacking boundaries and transport in bilayer graphene.
San-Jose P, Gorbachev RV, Geim AK, Novoselov KS, and Guinea F.
Nano Letters 14, 2052 (2014).

109 Complex chiral colloids and surfaces via high-index off-cut silicon.
McPeak KM, van Engers CD, Blome M, Park JH, Burger S, Gosalvez MA, Faridi A, Ries YR, Sahu A, and Norris, DJ.
Nano Letters 14, 2934 (2014).

110 Co nanodot arrays grown on a $GdAu_2$ template: substrate/nanodot antiferromagnetic coupling.
Fernández L, Blanco-Rey M, Ilyn M, Vitali L, Magaña A, Correa A, Ohresser P, Ortega JE, Ayuela A, and Schiller F.
Nano Letters 14, 2977 (2014).

111 Probing the site-dependent kondo response of nanostructured graphene with organic molecules.
Garnica M, Stradi D, Calleja F, Barja S, Diaz C, Alcami M, Arnau A, de Parga ALV, Martin F, and Miranda R.
Nano Letters 14, 4560 (2014).

112 Tunable plasmon modes in single silver nanowire optical antennas characterized by far-field microscope polarization spectroscopy.
Fu M, Qian LH, Long H, Wang K, Lu PX, Rakovich YP, Hetsch F, Susha AS, and Rogach AL.
Nanoscale 6, 9192 (2014).

113 Optical properties and sensing in plexcitonic nanocavities: from simple molecular linkers to molecular aggregate layers.
Perez-Gonzalez O, Zabala N, and Aizpurua J .
Nanotechnology 25, 035201 (2014).

114 Strong ferromagnetism at the surface of an antiferromagnet caused by buried magnetic moments.
Chikina A, Hoppner M, Seiro S, Kummer K, Danzenbacher S, Patil S, Generalov A, Guttler M,Kucherenko Y, Chulkov EV, Koroteev YM, Kopernik K, Geibel C, Shi M, Radovic M, Laubschat C, and Vyalikh DV.
Nature Communications 5, 3171 (2014).

115 Determining the polarization state of an extreme ultraviolet free-electron laser beam using atomic circular dichroism.
Mazza T, Ilchen M, Rafipoor AJ, Callegari C, Finetti P, Plekan O, Prince KC, Richter R, Danailov MB, Demidovich A, De Ninno G, Grazioli C, Ivanov R, Mahne N, Raimondi L, Svetina C, Avaldi L, Bolognesi P, Coreno M, O'Keeffe P, Di Fraia M, Devetta M, Ovchare
Nature Communications 5, 3648 (2014).

116 Chemical control of electrical contact to sp(2) carbon atoms.
Frederiksen T, Foti G, Scheurer F, Speisser V, and Schull G.
Nature communications 5, 3659 (2014).

117 Graphitic nanostripes in silicon carbidee surfaces created by swift heavy ion irradiation.
Ochedowski O, Osmani O, Schade M, Bussmann BK, Ban-d'Etat B, Lebius H, and Schleberger M.
Nature Communications 5, 3913 (2014).

118 Threading plasmonic nanoparticle strings with light.
Herrmann LO, Valev VK, Tserkezis C, Barnard JS, Scherman OA, Aizpurua J, and Baumberg JJ.
Nature Communications 5, 4568 (2014).

119 Local determination of the amount of integration of an atom into a crystal surface.
Volgmann K, Gawronski H, Zaum C, Rusina GG, Borisova SD, Chulkov EV, and Morgenstern K.
Nature Communications 5, 5089 (2014).

120 Strong coupling of single emitters interacting with phononic infrared antennae.
Esteban R, Aizpurua J, and Bryant GW.
New Journal of Physics 16, 013052 (2014).

121 Magneto-optical Kerr effect in resonant subwavelength nanowire gratings.
Marinchio H, Carminati R, Garcia-Martin A, and Saenz JJ.
New Journal of Physics 16, 015007 (2014).

122 One-dimensional potential for image-potential states on graphene.
de Andres PL, Echenique PM, Niesner D, Fauster TH, and Rivacoba A.
New Journal of Physics 16, 023012 (2014).

123 A chemically inert Rashba split interface electronic structure of $C_{60}$, FeOEP and PTCDA on $BiAg_2$/Ag(111) substrates.
Cottin MC, Lobo-Checa J, Schaffert J, Bobisch CA, Moller R, Ortega JE, and Walter AL.
New Journal of Physics 16, 045002 (2014).

124 Helmholtz Fermi surface harmonics: an efficient approach for treating anisotropic problems involving Fermi surface integrals.
Eiguren A and G. Gurtubay I.
New Journal of Physics 16, 063014 (2014).

125 Quantum ricochets: surface capture, release and energy loss of fast ions hitting a polar surface at grazing incidence.
Lucas AA, Sunjic M, Benedek G, and Echenique PM.
New Journal of Physics 16, 063015 (2014).

126 The gigantic Rashba effect of surface states energetically buried in the topological insulator $Bi_2Te_2Se$.
Miyamoto K, Okuda T, Nurmamat M, Nakatake M, Namatame H, Taniguchi M, Chulkov EV, Kokh KA, Tereshchenko OE, and Kimura A.
New Journal of Physics 16, 065016 (2014).

127 Giant diamagnetism of gold nanorods.
Hernando A, Ayuela A, Crespo P, and PM Echenique PM.
New Journal of Physics 16, 073043 (2014).

128 Relativistic force between fast electrons and planar targets.
Rivacoba A, and Zabala N.
New Journal of Physics 16, 073048 (2014).

129 Defect and structural imperfection effects on the electronic properties of BiTeI surfaces.
Fiedler S, El-Kareh L, Eremeev SV, Tereshchenko OE, Seibel C, Lutz P, Kokh KA, Chulkov EV, Kuznetsova TV, Grebennikov VI, Bentmann H, Bode M, and Reinert F.
New Journal of Physics 16, 075013 (2014).



130 Acoustic plasmons in extrinsic free-standing graphene.
Pisarra M, Sindona A, Riccardi P, Silkin VM, and Pitarke JM.
New Journal of Physics 16, 083003 (2014).

131 Electronic properties of graphene grain boundaries.
Ayuela A, Jaskolski W, Santos H, and Chico L.
New Journal of Physics 16, 083018 (2014).

132 Germanene: a novel two-dimensional germanium allotrope akin to graphene and silicene.
Dávila ME, Xian L, Cahangirov S, Rubio A, and Le Lay G.
New Journal of Physics 16, 095002 (2014).

133 Superspin glass phase and hierarchy of interactions in multiferroic $PbFe_{1/2}Sb_{1/2}O_3$: An analog of ferroelectric relaxors?
Laguta VV, Stephanovich VA, Savinov M, Marysko M, Kuzian RO, Kondakova IV, Olekhnovich NM,Pushkarev AV, Radyush YV, Raevski IP, Raevskaya SI, and Prosandeev SA.
New Journal of Physics 16, 113041 (2014).

134 Metallic thin films on stepped surfaces: lateral scattering of quantum well states.
Schiller F, Abd El-Fattah ZM, Schirone S, Lobo-Checa J, Urdanpilleta M, Ruiz-Oses M, Cordon J, Corso M, Sanchez-Portal D, Mugarza A, and Ortega JE.
New Journal of Physics 16, 123025 (2014).

135 Trajectory-dependent energy loss for swift He atoms axially scattered off a silver surface.
Rubiano CAR, Bocan GA, Juaristi JI, and Gravielle MS.
Nuclear Instruments and Methods in Physics Research Section B-beam Interactions with Materials and Atoms 340, 15 (2014).

136 Effects of pumping wavelength and pump density on the random laser performance of stoichiometric Nd crystal powders.
Azkargorta J, Iparraguirre I, Bettinelli M, Cavalli E, Barredo-Zuriarrain M, Garcia-Revilla S, Balda R, Fernandez J.
Optics Express 22, 27365 (2014)

137 Optical response of threaded chain plasmons: from capacitive chains to continuous nanorods.
Tserkezis Ch, Herrmann LO, Valev VK, Baumberg JJ, and Javier Aizpurua J.
Optics Express, 22, 23851 (2014).

138 Molecular dipole, dye structure and electron lifetime relationship in efficient dye sensitized solar cells based on donor-pi-acceptor organic sensitizers.
Climent C, Cabau L, Casanova D, Wang P, and Palomares E.
Organic Electronics 15, 3162 (2014).

139 Optical response of metallic nanoparticle heteroaggregates with subnanometric gaps.
Tserkezis Ch, Taylor RW, Beitner J, Esteban R, Baumberg JJ, and Aizpurua J.
Particle & Particle Systems Characterization 31, 152 (2014).

140 Gold spiky nanodumbbells: anisotropy in gold nanostars.
Novikov SM, Sánchez-Iglesias A, Schmidt MK, Chuvilin A, Aizpurua J, Grzelczak M, and Liz-Marzán LM.
Particle & Particle Systems Characterization 31, 77 (2014).

141 PFO-BPy solubilizers for SWNTs: Modelling of polymers from oligomers.
Glanzman LN, Mowbray DJ, and Rubio A.
Physica Status Solidi B-Basic Solid Sate Physics 251, 2407 (2014).

142 Theoretical electron energy loss spectroscopy of isolated graphene.
Mowbray DJ.
Physica Status Solidi B-Basic Solid State Physics 251, 2509 (2014).

143 Huge anharmonic effects in superconducting hydrides and transition metal dichalcogenides.
Errea I, Calandra M, and Mauri F.
Physica Status Solidi B-Basic Solid State Physics 251, 2556 (2014).

144 Intensity-voltage low-energy electron microscopy for functional materials characterization.
Flege JI and Krasovskii EE.
Physica Status Solidi-Rapid Research Letters 8, 463 (2014).

145 Tetrel bond–σ-hole bond as a preliminary stage of the $S_N2$ reaction.
Grabowski SJ.
Physical Chemistry Chemical Physics 16, 1824 (2014).

146 Mapping the affinity of aluminum(III) for biophosphates: interaction mode and binding affinity in 1:1 complexes.
Luque NB, Mujika JI, Rezabal E, Ugalde JM, and Lopez X.
Physical Chemistry Chemical Physics 16, 20107 (2014).

147 Structure, fragmentation patterns, and magnetic properties of small cobalt oxide clusters.
Aguilera-del-Toro RH, Aguilera-Granja F, Vega A and Balbá LC.
Physical Chemistry Chemical Physics 16, 21732 (2014).

148 Dynamics of supercooled water in a biological model system of the amino acid L-lysine.
Cerveny S, and Swenson J.
Physical Chemistry Chemical Physics 16, 22382 (2014).

149 Topological reaction sites – very strong chalcogen bonds.
Alikhani ME, Fuster F, Madebène B, and Grabowski SJ.
Physical Chemistry Chemical Physics 16, 2430 (2014).

150 Red-shifting the optical response of firefly oxyluciferin with group 15/16 substitutions.
Milne, BF.
Physical Chemistry Chemical Physics 16, 24971 (2014).

151 Polymorphic MnAs nanowires of a magnetic shape memory alloy.
Echeverria-Arrondo C, Perez-Conde J, and Ayuela A.
Physical Chemistry Chemical Physics 16, 5649 (2014).

152 Unveiling mode-selected electron–phonon interactions in metal films by helium atom scattering.
Benedek G, Bernasconi M, Bohnen KP, Campin D, Chulkov EV, Echenique PM, Heid R,
Sklyadneva IYu, and Toennies JP.
Physical Chemistry Chemical Physics 16, 7159 (2014).

153 Polarization control of metal-enhanced fluorescence in hybrid assemblies of photosynthetic complexes and gold nanorods.
Bujak L, Olejnik M, Brotosudarmo THP, Schmidt MK, Czechowski N, Piatkowski D, Aizpurua J,
Cogdell RJ, Heisse W, and Mackowski S.
Physical Chemistry Chemical Physics 16, 9015 (2014).

154 Pulse-delay effects in the angular distribution of near- threshold EUV plus IR two-photon ionization of Ne.
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, Miron C, Nagasono M, Togashi T, Yabashi M,
Ishikawa KL, Kazansky AK, Kabachnik NM, and Ueda K.
Physical Review A 89, 013415 (2014).

155 Energy-loss contribution to grazing scattering of fast He atoms from a silver surface.
Rubiano CAR, Bocan GA, Juaristi JI, and Gravielle, MS.
Physical Review A 89, 032706 (2014).

156 Effect of long-range spatial correlations on the lifetime statistics of an emitter in a two-dimensional disordered lattice.
de Sousa N, Sáenz JJ, García-Martín A, Froufe-Pérez LS, and Marqués MI.
Physical Review A 89, 063830 (2014).

157 Quantum-electrodynamical density-functional theory: Bridging quantum optics and electronic-structure theory.
Ruggenthaler M, Flick J, Pellegrini C, Appel H, Tokatly IV, and Rubio A.
Physical Review A 90, 012508 (2014).

158 Theoretical study of pulse delay effects in the photoelectron angular distribution of near-threshold EUV plus IR two-photon ionization of atoms.
Ishikawa KL, Kazansky AK, Kabachnik NM and Ueda K.
Physical Review A 90, 023408 (2014).

159 Local reduced-density-matrix-functional theory: Incorporating static correlation effects in Kohn-Sham equations.
Lathiotakis NN, Helbig N, Rubio A, and Gidopoulos NI.
Physical Review A 90, 032511 (2014).

160 Attosecond near-threshold photoionization in a strong laser field.
Kazansky AK, Bozhevolnov AV, Sazhina IP, and Kabachnik NM.
Physical Review A 90, 033409 (2014).

161 Time-dependent density-functional theory of strong-field ionization of atoms by soft x rays.
Crawford-Uranga A, De Giovannini U, Rasanen E, Oliveira MJT, Mowbray DJ, Nikolopoulos M,
Karamatskos ET, Markellos D, Lambropoulos P, Kurth S, and Rubio A.
Physical Review A 90, 033412 (2014).

162 Breakdown of the Peierls substitution for the Haldane model with ultracold atoms.
Ibanez-Azpiroz J, Eiguren A, Bergara A, Pettini G, and Modugno M.
Physical Review A 90, 033609 (2014).

163 Optimal control of high-harmonic generation by intense few-cycle pulses.
Solanpää J, Budagosky JA, Shvetsov-Shilovski NI, Castro A, Rubio A, and Rasanen E.
Physical Review A 90, 053402 (2014).

164 Probing two-dimensional Anderson localization without statistics.
Leseur O, Pierrat R, Sáenz JJ, and Carminati R.
Physical Review A 90, 053827 (2014).

165 Comment on "Weyl fermions and the anomalous Hall effect in metallic ferromagnets".
Vanderbilt D, Souza I, and Haldane FDM.
Physical Review B (Condensed Matter and Materials Physics) 89, 117101 (2014).

166 Energy bands in graphene: comparison between the tight-binding model and ab initio calculations.
Kogan E, Nazarov VU, Silkin VM, and Kaveh M.
Physical Review B (Condensed Matter and Materials Physics) 89, 165430 (2014).

167 Atomic relaxations at the (0001) surface of $Bi_2Se_3$ single crystals and ultrathin films.
Roy S, Meyerheim HL, Mohseni K, Ernst A, Otrokov MM, Vergniory MG, Mussler G, Kampmeier D, Grützmacher D, Tusche C, Schneider J, Chulkov EV, and Kirschner J.
Physical Review B (Condensed Matter and Materials Physics) 90, 155456 (2014).

168 Effects of 5d electrons and spin-orbit interaction on the characteristics of bulk plasmons in lead.
Zubizarreta X, Silkin VM, and Chulkov EV.
Physical Review B (Condensed Matter and Materials Physics) 90, 165121 (2014).

170 Ab initio lattice dynamics and electron-phonon coupling of Bi(111).
Alcantara Ortigoza M, Sklyadneva IYu, Heid R, Chulkov EV, Rahman TS, Bohnen KP, and chenique PM.
Physical Review B (Condensed Matter and Materials Physics) 90, 195438 (2014).

171 Magnetism and morphology of Co nanocluster superlattices on $GdAu_2$/Au(111)-(13×13).
Cavallin A, Fernande L, Ilyn M, Magana A, Ormaza M, Matena M, Vitali L, Ortega JE, Grazioli C, hresser P, Rusponi S, Brune H, and Schiller F.
Physical Review B (Condensed Matter and Materials Physics) 90, 235419 (2014).

172 Nontrivial spin structure of graphene on Pt(111) at the Fermi level due to spin-dependent hybridization
Klimovskikh II, Tsirkin SS, Rybkin AG, Rybkina AA, Filianina MV, Zhizhin EV, and Chulkov EV, and Shikin AM.
Physical Review B (Condensed Matter and Materials Physics) 90, 235431 (2014).

173 Magnetic interactions in disordered perovskite PbFe1/2Nb1/2O3 and related compounds: Dominance of nearest-neighbor interaction.
Kuzian RO, Kondakova IV, Dare AM, and Laguta, VV.
Physical Review B 89, 024402 (2014).

174 Theory of action spectroscopy for single-molecule reactions induced by vibrational excitations with STM.
Frederiksen T, Paulsson M, and Ueba H.
Physical Review B 89, 035427 (2014).

175 Manifestation of a spin-splitting field in a thermally biased Josephson junction.
Bergeret FS, and Giazotto F.
Physical Review B 89, 054505 (2014).

176 Magnetic fluctuations in topological insulators with ordered magnetic adatoms: Cr on $Bi_2Se_3$ from first principles.
Chotorlishvili L, Ernst A, Dugaev VK, Komnik A, Vergniory MG, Chulkov EV, and Berakdar J.
Physical Review B 89, 075103 (2014).

177 Bulk and surface electron dynamics in a p-type topological insulator $SnSb_2Te_4$.
Niesner D, Otto S, Hermann V, Fauster TH, Menshchikova TV, Eremeev SV, Aliev ZS, Amiraslanov IR, Babanly MB, Echenique PM, and Chulkov EV.
Physical Review B 89, 081404(R) (2014).

178 Efficient calculation of inelastic vibration signals in electron transport: Beyond the wide-band approximation.
Lu JT, Christensen RB, Foti G, Frederiksen T, Gunst T, and Brandbyge M.
Physical Review B 89, 081405 (2014).

179 Ab initio analysis of plasmon dispersion in sodium under pressure.
Ibañez-Azpiroz J, Rousseau B, Eiguren A, and Bergara A.
Physical Review B 89, 085102 (2014).

180 Many-body interactions and Rashba splitting of the surface state on Cu(110).
Jiang J, Tsirkin SS, Shimada K, Iwasawa H, Arita M, Anzai H, Namatame H, Taniguchi M, Sklyadneva IYu, Heid R, Bohnen KP, Echenique PM, and Chulkov EV.
Physical Review B 89, 085404 (2014).

181 Electronic and spin structure of the topological insulator $Bi_2Te_{2.4}Se_{0.6}$.
Shikin AM, Klimovskikh II, Eremeev SV, Rybkina AA, Rusinova MV, Rybkin AG, Zhizhin EV, Sánchez-Barriga J, Varykhalov A, Rusinov IP, Chulkov EV, Kokh KA, Golyashov VA, Kamyshlov V, and Tereshchenko OE.
Physical Review B 89, 125416 (2014).

182 Spin-orbit coupling as a source of long-range triplet proximity effect in superconductor-ferromagnet hybrid structures.
Bergeret FS, and Tokatly IV.
Physical Review B 89, 134517 (2014).

183 Fully self-consistent GW and quasiparticle self-consistent GW for molecules.
Koval P, Foerster D, and Sanchez-Portal D.
Physical Review B 89, 155417 (2014).

184 Influence of the surface band structure on electron emission spectra from metal surfaces.
Archubi CD, Faraggi MN, Silkin VM, and Gravielle MS.
Physical Review B 89, 155421 (2014).

185 Exchange interaction and its tuning in magnetic binary chalcogenides.
Vergniory MG, Otrokov MM, Thonig D, Hoffmann M, Maznichenko IV, Geilhufe M, Zubizarreta X, Ostanin S, Marmodoro A, Henk J, Hergert W, Mertig I, Chulkov EV, and Ernst A.
Physical Review B 89, 165202 (2014).

186 Combined effect of stacking and magnetic field on plasmon excitations in bilayer graphene.
Wu JY, Gumbs G, and Lin MF.
Physical Review B 89, 165407 (2014).

187 Role of surface passivation in the formation of Dirac states at polar surfaces of topological crystalline insulators: The case of SnTe(111).
Eremeev SV, Koroteev YM, Nechaev IA, and Chulkov EV.
Physical Review B 89, 165424 (2014).

188 Using surface plasmonics to turn on fullerene's dark excitons.
Despoja V, and Mowbray DJ.
Physical Review B 89, 195433 (2014).

189 Silicene versus two-dimensional ordered silicide: atomic and electronic structure of Si-(root 19x root 19)R23.4 degrees/Pt(111).
Svec M, Hapala P, Ondracek M, Merino P, Blanco-Rey M, Mutombo P, Vondracek M, Polyak Y, Chab V, Martin-Gago JA, and Jelinek P.
Physical Review B 89, 201412 (2014).

190 Plasmaron excitations in p(2 x 2)-K/graphite.
Chis V, Silkin VM, and Hellsing B.
Physical Review B 89, 205429 (2014).

191 Revealing Hofstadter spectrum for graphene in a periodic potential.
Gumbs G, Iurov A, Huang D, and Zhemchuzhna L.
Physical Review B 89, 241407(R) (2014).

192 Atomic structure of the root 3 x root 3 phase of silicene on Ag(111).
Cahangirov S, Ozcelik VO, Xian LD, Avila J, Cho S, Asensio MC, Ciraci S, and Rubio A.
Physical Review B 90, 035448 (2014).

193 Exchange integrals in Mn- and Co-doped II-VI semiconductors.
Savoyant A, D'Ambrosio S, Kuzian RO, Dare AM, and Stepanov A.
Physical Review B 90, 075205 (2014).

194 Benchmarking van der Waals functionals with noncontact RPA calculations on graphene-Ag(111).
Loncaric I, and Despoja V.
Physical Review B 90, 075414 (2014).

195 Plasmons in a superlattice of fullerenes or metallic shells.
Balassis A, and Gumbs G.
Physical Review B 90, 075431 (2014).

196 Spectroscopy and dynamics of unoccupied electronic states of the topological insulators $Sb_2Te_3$ and $Sb_2Te_2S$.
Reimann J, Gudde J, Kuroda K, Chulkov EV, and Hofer U.
Physical Review B 90, 081106 (2014).

197 First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory.
Caruso F, Atalla V, Ren XG, Rubio A, Scheffler M, and Rinke P.
Physical Review B 90, 085141 (2014).

198 Silicite: The layered allotrope of silicon.
Cahangirov S, Ozcelik VO, Rubio A, and Ciraci S.
Physical Review B 90, 085426 (2014).

199 Microscopic origin of the relativistic splitting of surface states.
Krasovskii, EE.
Physical Review B 90, 115434 (2014).

200 High-energy collective electronic excitations in layered transition-metal dichalcogenides.
Cudazzo P, Ruotsalainen KO, Sahle CJ, Al-Zein A, Berger H, Navarro-Moratalla E, Huotari S, Gatti M,and Rubio A.
Physical Review B 90, 125125 (2014).

201 How disorder affects the Berry-phase anomalous Hall conductivity: a reciprocal-space analysis.
Bianco R, Resta R, and Souza I.
Physical Review B 90, 125153 (2014).

202 On-surface synthesis of a two-dimensional porous coordination network: Unraveling adsorbate interactions.
Matena M, Bjork J, Wahl M, Lee TL, Zegenhagen J, Gade LH, Jung TA, Persson M, and Stohr M.
Physical Review B 90, 125408 (2014).

203 Lieb-Mattis ferrimagnetic superstructure and superparamagnetism in Fe-based double perovskite multiferroics.
Kuzian RO, Laguta VV, and Richter J.
Physical Review B 90, 134415 (2014)

204 Ab initio nanoplasmonics: The impact of atomic structure.
Zhan P, Feist J, Rubio A, Garcia-Gonzalez P, and Garcia-Vidal FJ.
Physical Review B 90, 161407 (2014).

205 Interplay between structure and electronic properties of layered transition-metal dichalcogenides: comparing the loss function of 1T and 2H polymorphs.
Cudazzo P, Gatti M, and Rubio A.
Physical Review B 90, 205128 (2014).

206 Superconducting pairing mediated by spin fluctuations from first principles.
Essenberger F, Sanna A, Linscheid A, Tandetzky F, Profeta G, Cudazzo P and Gross EKU.
Physical Review B 90, 214504 (2014).

207 Spin-valley relaxation and quantum transport regimes in two-dimensional transition-metal dichalcogenides.
Ochoa H, Finocchiaro F, Guinea F, and Fal'ko VI.
Physical Review B 90, 235429 (2014).

208 Local control of the excitation of surface plasmon polaritons by near-field magneto-optical Kerr effect.
Vincent R, Marinchio H, Saenz JJ, and Carminati R.
Physical Review B 90, 241412 (2014).

209 Theory of coupled spin-charge transport due to spin-orbit interaction in inhomogeneous two-dimensional electron liquids.
Shen K, Raimondi R, and Vignale G.
Physical Review B 90, 245302 (2014).

210 Predicted very large thermoelectric effect in ferromagnet-superconductor junctions in the presence of a spin-splitting magnetic field.
Ozaeta A, Virtanen P, Bergeret FS, and Heikkila TT.
Physical Review Letters 112, 057001 (2014).

211 Spin texture of $Bi_2Se_3$ thin films in the quantum tunneling limit.
Landolt G, Schreyeck S, Eremeev SV, Slomski B, Muff S, Osterwalder J, Chulkov EV, Gould C, Karczewski G, Brunner K, Buhmann H, Molenkamp LW, and Dil JH.
Physical Review Letters 112, 057601 (2014).

212 Spin-Dependent Electron Scattering at Graphene Edges on Ni(111).
Garcia-Lekue A, Balashov T, Olle M, Ceballos G, Arnau A, Gambardella P, Sanchez-Portal D, and Mugarza A.
Physical Review Letters 112, 066802 (2014).

213 Electronic friction dominates hydrogen hot-atom relaxation on Pd(100).
Blanco-Rey M, Juaristi JI, Díez Muiño R, Busnengo HF, Kroes GJ, and Alducin M.
Physical Review Letters 112, 103203 (2014).

214 Self-assembly of bicomponent molecular monolayers: adsorption height changes and their consequences.
Goiri E, Matena M, El-Sayed A, Lobo-Checa J, Borghetti P, Rogero C, Detlefs B, Duvernay J, Ortega JE, and de Oteyza DG.
Physical Review Letters 112, 117602 (2014).

215 Role of physisorption states in molecular scattering: a semilocal density-functional theory study on $O_2$/Ag(111).
Goikoetxea I, Meyer J, Juaristi JI, Alducin M, and Reuter K.
Physical Review Letters 112, 156101 (2014).

216 Stable single-layer honeycomblike structure of silica.
Ozcelik VO, Cahangirov S, and Ciraci S.
Physical Review Letters 112, 246803 (2014).

217 Surface strain improves molecular adsorption but hampers dissociation for $N_2$ on the Fe=W(110) surface.
Goikoetxea I, Juaristi JI, Díez Muiño R, and Alducin M.
Physical Review Letters 113, 066103 (2014).

218 Quantum spin hall effect in two-dimensional crystals of transition-metal dichalcogenides.
Cazalilla MA, Ochoa H, and Guinea F.
Physical Review Letters 113, 077201 (2014).

219 Polymer chain dynamics: evidence of nonexponential mode relaxation using thermally stimulated depolarization current techniques.
Arrese-Igor S, Alegria A, and Colmenero J.
Physical Review Letters 113, 078302 (2014).

220 Correlated electron-nuclear dynamics with conditional wave functions.
Albareda G, Appel H, Franco I, Abedi A, and Rubio A.
Physical Review Letters 113, 083003 (2014).

221 Tuning the Dirac point position in $Bi_2Se_3$(0001) via surface carbon doping.
Roy S, Meyerheim HL, Ernst A, Mohseni K, Tusche C, Vergniory MG, Menshchikova TV, Otrokov MM,Ryabishchenkova AG, Aliev ZS, Babanly MB, Kokh KA, Tereshchenko OE, Chulkov EV, Schneider J, and Kirschner J.
Physical Review Letters 113, 116802 (2014).

222 Anisotropic dispersion and partial localization of acoustic surface plasmons on an atomically stepped surface: Au(788).
Smerieri M, Vattuone L, Savio L, Langer T, Tegenkamp C, Pfnur H, Silkin VM, and Rocca M.
Physical Review Letters 113, 186804 (2014).

223 Instantaneous band gap collapse in photoexcited monoclinic $VO_2$ due to photocarrier doping.
Wegkamp D, Herzog M, Xian L, Gatti M, Cudazzo P, McGahan CL, Marvel RE, Haglund RF, Rubio A, Wolf M, Stahler J.
Physical Review Letters 113, 216401 (2014).

224 How many-body effects modify the van der Waals interaction between graphene sheets.
Dobson JF, Gould T, and Vignale G.
Physical Review X 4, 021040 (2014).

225 Unconventional phase diagram for six heavy rare earth metals showing melting plus magnetic transitions versus the de Gennes factor.
Ayuela A, and March NH.
Physics and Chemistry and Chemistry of Liquids 52, 650 (2014).

226 The key role of electron-nuclear potential energy in determining the ground-state energy of inhomogeneous electron liquids in both real and model atoms.
Amovilli C, and March NH.
Physics and Chemistry of Liquids 52, 576 (2014).

227 Crucial combinations of critical exponents for liquids-vapour and ferromagnetic second-order phase transitions.
March NH.
Physics and Chemistry of Liquids 52, 697 (2014).

228 Weizsacker inhomogeneity kinetic energy term for the inhomogeneous electron liquid characterising some 30 homonuclear diatomic molecules at equilibrium and insight into Teller's theorem in Thomas-Fermi statistical theory.
Piris M, and March NH.
Physics and Chemistry of Liquids 52, 804 (2014).

229 Generalisation of Zhang's predictions for the critical exponents of the 3d Ising model if alpha not equal 0.
March NH.
Physics and Chemistry of Liquids 52, 815 (2014).

230 Inclusion of an applied magnetic field of arbitrary strength in the Ising model.
March NH.
Physics Letters A 378, 2295 (2014).

231 Ab initio calculations of the electron-phonon interaction and characteristics of large polarons in rutile and anatase.
Zhukov VP, and Chulkov EV.
Physics of the Solid State 56, 1302 (2014).

232 Dynamic study of polystyrene-block-poly(4-vinylpyridine) copolymer in bulk and confined in cylindrical nanopores.
Maiz J, Zhao W, Gu Y, Lawrence J, Arbe A, Alegria A, Emrick T, Colmenero J, Russell T, and Mijangos C.
Polymer 55, 4057 (2014).

233 Zwitterionic polymerization of glycidyl monomers to cyclic polyethers with $B(C_6F_5)_3$.
Asenjo-Sanz I, Veloso A, Miranda JI, Pomposo JA, and Barroso-Bujans F.
Polymer Chemistry 5, 6905 (2014).

234 Ultracold Fermi gases with emergent SU(N) symmetry.
Cazalilla MA, and Rey AM.
Reports on Progress in Physics 77, 124401 (2014).

235 Coherent ultrafast charge transfer in an organic photovoltaic blend.
Falke SM, Rozzi CA, Brida D, Maiuri M, Amato M, Sommer E, De Sio A, Rubio A, Cerullo G, Molinari E, and Lienau C.
Science 344, 6187 (2014).

236 A strategy to create spin-split metallic bands on silicon using a dense alloy layer.
Gruznev DV, Dimitry V, Bondarenko LV, Matetskiy AV, Yakovlev AA, Tupchaya AY, Eremeev SV, Chulkov EV, Chou JP, Wei CM, Lai MY, Wang YL, Zotov AV, and Saranin AA.
Scientific Reports 4, 4742 (2014).

237 Novel superconducting skutterudite-type phosphorus nitride at high pressure from first-principles calculations.
Raza Z, Errea I, Oganov AR, and Saitta AM.
Scientific Reports 4, 5889 (2014)

238 Spin-helical Dirac states in graphene induced by polar-substrate surfaces with giant spin-orbit interaction: a new platform for spintronics.
Eremeev EV, Nechaev IA, Echenique PM, and Chulkov EV.
Scientific Reports 4, 6900 (2014).

239 Gold nanorods with sub-nanometer separation using cucurbit[n]uril for SERS applications.
Jones ST, Taylor RW, Esteban R, Abo-Hamed EK, Bomans PHH, N, Sommerdijk NAJM, Aizpurua J, Baumberg JJ and Scherman OA.
Small 10, 4298 (2014).

240 Multi-orthogonal folding of single polymer chains into soft nanoparticles.
Lo Verso F, Pomposo JA, Colmenero J, and Moreno AJ.
Soft Matter 10, 4813 (2014).

241 Single-chain nanoparticles vs. star, hyperbranched and dendrimeric polymers: Effect of the nanoscopic architecture on the flow properties of diluted solutions.
Perez-Baena I, Moreno AJ, Colmenero J, and Pomposo JEA.
Soft Matter 10, 9454 (2014).

242 Coulomb edge effects in graphene nanoribbons.
Jaskolski W, and Ayuela A.
Solid State Communications 196, 1 (2014).

243 Accounting for the thickness dependence of the T-g in supported PS films via the volume holes diffusion model.
Boucher VM, Cangialosi D, Alegria A, and Colmenero J.
Thermochimica Acta 575, 233 (2014).

244 AFM based dielectric spectroscopy: Extended frequency range through excitation of cantilever higher eigenmodes.
Miccio LA, Kummali MM, Schwartz GA, Alegria A, and Colmenero J.
Ultramicroscopy 146, 55 (2014).

# Researchers

## Fellows Gipuzkoa

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

Dr. Maia Garcia 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
Asociación de Investigación Material Physics Center (MPC), Donostia-San Sebastián, Spain
25/11/2013–Present
Development of MBPT with localized orbitals.

Dr. Dimas Garcia de Oteyza Feldermann
Centro de Fisica de Materiales CSIC-UPV/EHU, Donostia-San Sebastián
01/05/2014–Present
Physical chemistry phenomena in organic materials and organic-inorganic interfaces.

Dr. Aitzol Garcia Etxarri
Stanford University, San Francisco, USA
01/11/2014–Present
Nanophotonics theory.

## Postdoctoral Positions

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 Beatriz Luque
Universidad Nacional de Córdoba, Argentina
01/11/2012–31/12/2014
Ab-initio quantum chemistry studies of seleno-L-cysteine on coinage metal surfaces.

Dr. Stepan Tsirkin
State University of Tomsk, Russia
06/12/2012–Present
Magnetic proximity effect in the layered structures.

Dr. Pablo Aguado Puente
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01/01/2013–31/12/2014
Coupling of ferroic nanoscale films with interfacial two dimensional electron gases in oxides.

Dr. Chang-Jin Lee
Boston College, USA
01/04/2013–26/03/2014
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–Present
Aimed at finding the much-needed link between structure and properties of polymers confined at sub-nanometer dimensions at both fundamental and practical levels via understanding, tuning, and, ultimately, controlling the properties of polymer-based graphene nanostructured matter.

Dr. Rubén González Moreno
Instituto de Ciencia de Materiales de Madrid, CSIC, Spain
01/07/2013–31/12/2014
Fabrication of curved single crystals.

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

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

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

Dr. Ion Errea Lope
Institut de Minéralogie et de Physique de Milieux Condensés, Université Pierre et Marie Curie, Paris, France
02/01–31/12/2014
Anharmonic free energies and phonon dispersions from the self-consistent harmonic approximation.

Dr. Marcos Gonçalves de Menezes
Universidade Federal Do Rio de Janeiro, Brasil
27/01–13/03/2014
Anomalous hall effect in metals and Chern insulators, and gyrotropic optical effects.

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

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

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

Dr. Yao Zhang
University of Science and Technology of China (USTC), Anhui, China
21/08–05/10/2014
Plasmon.enhanced infrared spectroscopies for molecular characterization.

Dr. Daniel Gosálbez Martínez
Centro de Física de Materiales and Universidad del País Vasco, Donostia- San Sebastián, Spain
15/09–31/12/2014
Weyl nodes in ferromagnetic bandstructures.

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

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

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

## Temporary Contract Positions

Dr. Irina Sklyadneva
Russian Academy of Sciences, Tomsk, Russia
14/05/2003–Present
Lattice dynamics and electron-phonon interaction in bulk materials and in ultrathin metal films. Electron-phonon interactions are of paramount importance for the correct description of the temperature dependence of quasiparticle dynamics. The goal of the present project is to study the electron-phonon coupling in ultrathin lead films, at bismuth and noble metal surfaces and in bismuth tellurohalides, layered polar semiconductors.

Dr. Laura Fernández Gómez-Recuero
Technische Universität Dresden (TU-Dresden), Germany
01/01–31/08/2014
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.



## PhD Students

Elisabeth Goiri Little
Facultad de Ciencias, UPV/EHU, Lejona, Spain
01/07/2010–28/02/2014
Tunneling microscopy and spectroscopy of molecules on metals at 1 K.

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

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

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

Aitzol Iturbe Beristain
UPV/EHU, Donostia-San Sebastián, Spain
01/10/2013–31/03/2014
Electron-phonon interaction in surfaces with strong spin-orbit interaction.

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

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

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

# Visiting Researchers

## Long visits

Prof. Godfrey Gumbs
Hunter College, The City University of New York, USA
07/01–07/02/2014
Plasmons in nanostructures.

Prof. Giorgio Benedek
Universitá degli Studi di Milano-Bicoca, Milan, Italy
09/01–28/02/2014, 09/09–01/11/2014
Surface phonons and phase transitions.

Dr. Nikolai Zaitcev
Philipps- Universität Marburg, Germany
24/01–04/04/2014
First principle electronic structure calculations of organic molecules absorbed on metallic surfaces.

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

Prof. Norman March
University of Antwerpen, Belgium
04/02–04/04/2014
Study of the role of exchange and correlation effects in both ground state density functional theory as well as excitation within time-dependent density-functional theory.

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

Dr. Bruce Milne
Centre for Computational Physics,
University of Coimbra, Coimbra, Portugal
08/02–08/05/2014, 03/11–12/12/2014
Theoretical spectroscopy of the light harvesting complex from green plants.

Dr. Ziya Aliyev
Baku State University, Azerbaijan
01/12/2013–28/05/2014, 02/10–30/12/2014
Materials physics of topological insulators.

Prof. Istvan Nagy
Technical University of Budapest, Hungary
03/01–01/02/2014
Various aspects of correlations in extended fermionic systems; spin-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Prof. Joseph R. Manson
Clemson University, Clemson, South Carolina, USA
12/02–17/03/2014, 02/10–12/11/2014
Theoretical studies of structure and dynamics of microscopic surfaces.

Prof. Vladimir Nazarov
Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan
21/02–21/03/2014
Time-dependent density-functional theory of particle-solid interactions.

Prof. Roman O. Kuzian
National Academy of Sciences of Ukranie, Kiev, Ukraine
01/03–30/04/2014, 01/11–23/12/2014
Photoemission from strongly correlated systems.

Prof. Giovanni Vignale
University of Missouri, Columbia, Missouri, USA
10/04/201420/06/2014
Condensed matter theory.

Dr. Mathias Ljunberg
Laboratoire ondes et matière d'Aquitaine (LOMA) - CNRS, Talence, France
16/04/201416/04/2016
First principles calculations of complex oxides.

Prof. Alexander Protogenov
Institute of Applied Physics of Russian Academy of Sciences, Nizhnii Novgorod, Russia
01/05/201431/05/2014
Transport properties of 3D topological insulators.

Prof. Peter Saalfrank
Institut für Chemie, Universität Postdam, Postdam-Golm, Germany
02/05/201431/07/2014
Elastic, inelastic, and reactive scattering of atoms and molecules from surfaces.

Francesco Ferrari (PhD Student)
Universitá Milano Bicocca, Milan, Italy
05/05/201430/11/2014
GW calculation of a molecule adsorbed on a titanium dioxide substrate.

Dr. Marisa Faraggi
Instituto de Astronomía y Fisica del Espacio IAFE (CONICET-UBA) Ciudad Autónoma de Buenos Aires, Argentina
12/05–11/07/2014
Study of electronic dynamics on transitions metals dichalcogenides (TMDC) and modelling of 2D metal-organic networks on metallic surfaces.

Dr. Sergey Eremeev
Institute of Strength Physics and Materials Sciences, Tomsk, Russia
01/06–29/08/2014
Electronic properties of topological insulators.

Prof. Vladimir Menshov
Russian Research Center "Kurchatov Institute", Moscow, Russia
02/06–31/08/2014
Magnetic impurities in digital alloys and topological insulators.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
03/06–31/07/2014, 15/12–15/01/2015
Nanostructure materials.

Marcos Dominguez Rivera (PhD Student)
Università di Trieste and CNR-IOM, Italy
09/06–01/08/2014
Structural and electronic coupling of organics poly and heteroaromatic molecules on inorganic surfaces of oxides and metals.

Prof. Jon Marcaide Osoro
Universidad de Valencia, Burjassot, Spain
16/06–11/09/2014
Radio astronomy.

Prof. Eugene Kogan
Bar-Ilan University, Ramat-Gan, Israel
16/06–23/07/2014
Electronic properties of graphene.

Prof. Luis Alberto Montero Cabrera
Facultad de Química, Universidad de la Habana, Cuba
20/06–20/07/2014
Molecular modeling of excited electronic states of nanoscopic systems.

Prof. Nikolay Kabachnik
Institut fur Experimentalphysik, Hamburg, Germany
01/07–30/09/2014
Study of Auger processes in gases and at solid surfaces within an attosecond streaking scheme.



Prof. Andrey Borisov
Université Paris Sud, France
01/07–31/08/2014
Time dependent density functional theory calculations to address the optical response of plasmonic systems.

Prof. Francisco Guinea Lopez
Instituto de Ciencia Materiales de Madrid-CSIC, Madrid, Spain
01/07–31/07/2014
Condensed matter physics.

Dr. Zakaria Abd El-Fattah
Faculty of Science, Al-Azhar University, Cairo, Egypt
01/07–30/09/2014
Angle resolved photoemission experiments in metallic nanostructures.

Dr. Marisol Alcántara Ortigoza
University of Central Florida, Orlando, Florida, USA
02/07–31/08/2014
Optical and electronic properties of transition-metal dichalcogenides.

Dr. Miguel Angel Cazalilla
National University of Singapore
15/07–15/08/2014
Strongly correlated systems, Bose Condensates, mesoscopic and low-dimensional systems in and out of equilibrium. Electronic excitations in surfaces and anisotropic systems.

Prof. Wlodzimierz Jaskólski
Institute of Physics Nicholas Copernicus University, Torun, Poland
20/07–30/09/2014
Study of quantum dot arrays and nanotube superlattices.

Kaiqiang Lin (PhD Student)
Xiamen University, Xiamen, Fujian Province, China
21/07–27/08/2014
Relation between near-field and far-field information in surface enhanced Raman spectroscopy and photoluminiscence of single gold nanorod.

Prof. Vladimir Kuznetsov
Tomsk State University, Tomsk, Russia
01/08–31/08/2014
Density functional methods in the theory of phase diagrams of alloys and in the Kondo effects.

Prof. Jeremy Baumberg
University of Cambridge, United Kingdom
01/08/201431/08/2014
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.

Dr. Vito Despoja
University of Zagreb, Croatia
01/08–30/09/2014
Plasmonics of intercalated monolayer and bilayer graphene.

Prof. Viktor Tugushev
National Research Center "Kurchatov Institute", Moscow, Russia
04/08–31/10/2014
Magnetism in superlattices and spintronics.

Dr. Peng Zhang
University of Science and Technology of China, Hefei, Anhui, China
18/08–13/01/2015
Morphokinetics: Morphology-based modeling of the growth kinetics of 2D materials.

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

Prof. Wolfgang Schattke
Universität Kiel, Germany
01/09–13/11/2014
Variational Quantum Montecarlo calculations of the electronic properties of solids and surfaces. Theory of photoemission in semiconductors and metals.

Dr. Tatiana Menshchikova
State University of Tomsk, Russia
01/09–28/11/2014
Excitations on surfaces with defects.

Prof. Vladlen Zhukov
Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia
01/09–28/11/2014
Electron dynamics in oxides: electron-electron and electron-phonon mechanisms of decay of excited electrons.

Dr. Igor Rusinov
State University of Tomsk, Russia
01/09–28/11/2014
Excitations on surfaces with defects.

Prof. Marijan Sunjic
University of Zagreb, Croatia
03/09–30/10/2014
Dynamical response and surface excitations in thin films.

Prof. Amand Lucas
FUNDP, Namur, Belgium
04/09–31/10/2014
Condensed matter physics, surface sciences, electronic and atomic structures of reduced dimensionality systems structural biology.

Romain Dupuis
CEMES/CNRS, Toulouse, France
08/09–09/12/2014
Cements and nanoadditions.

Dr. José Surga Diaz
Petroleos de Venezuela S.A. PDVSA-INTEVEP, Venezuela
15/09–12/12/2014
Cements under presure and temperature.

Dr. Carlos Echeverria Arrondo
Facultad de Ciencia y Tecnología, UPV/EHU, Bilbao, Spain
15/09–28/02/2015
Calculations on magnetic properties for ZnO nanoparticles.

Prof. Raffaele Resta
Università di Trieste, Trieste, Italy
12/10–16/12/2014
Computational modelling of materials physics.

Dr. Chang-Jin Lee
KITECH, Korea Institute for Industrial Technology, Cheonan, Republic of Korea
15/10–15/12/2014
Electronic excitations and many-body effects in solids, surfaces, and nanostructures.

Prof. Julio A. Alonso Martín
Universidad de Valladolid, Spain
20/10–20/11/2014
Electronic structure of carbon-based materials.

Iker Gallardo Arrieta (PhD Student)
Facultad de Ciencia y Tecnología, UPV/EHU, Bilbao, Spain
20/10–20/01/2015
Sistematic study of electronic and magnetic properties of metal-organic coordination networks and the effects of strain on its systems.

Dr. Yury Koroteev
Tomsk State University, Russia
23/10–21/12/2014
First principles calculations of the electronic structure.

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

## Short visits

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
02/01–16/01/2014, 20/04–27/04/2014
Nanostructure materials.

Prof. Larry Glasser
Clarkson University, Potsdam, New York, USA
12/01–18/01/2014
Mathematical physics applied to condensed matter.

Dr. Iñigo Liberal Olleta
Universidad Pública de Navarra, Pamplona, Spain
21/01–21/01/2014
Optical forces produced by localized sources.

Prof. Iñigo Ederra Urzainqui
Universidad Pública de Navarra, Pamplona, Spain
21/01–21/01/2014
Optical forces produced by localized sources.

Dr. Dario Bercioux
Dahlem Center for Complex Quantum Systems, Freie Universitaet Berlin, Germany
22/01–26/01/2014, 17/08–25/08/2014
Quantum transport in low dimensional systems.

Dr. Marta Pelc
Instituto de Ciencia de Materiales, CSIC, Madrid, Spain
25/01–16/02/2014
Graphene and carbon nanotubes.

Prof. Jean-Pierre Luminet
Observatoire de Paris, LUTH, Meudon, France
30/01–30/01/2014
Recent developments in black holes physics and astrophysics.

Prof. Gaspar Armelles
Instituto de Microelectrónica de Madrid, IMM (CNM-CSIC), Madrid, Spain
05/02–06/02/2014
Magnetoplasmonics.

Dr. Victor Morales Florez
Universidad de Sevilla, Spain
05/02–07/02/2014
C-S-H gel cements.

Prof. Andreas Otto
Universität Düsseldorf, Germany
16/02–23/02/2014, 26/03–04/04/2014
Raman spectroscopy.

Dr. Luca Bergamini
Università di Modena e Reggio Emilia, Modena, Italy
19/02–22/02/2014
Plasmonic properties of metal-nanoparticles interacting with molecules.

Prof. Salvador Miret Artes
Instituto de Física Fundamental, CSIC, Madrid, Spain
24/02–27/02/2014, 14/10–16/10/2014
Theory of surface diffusion.

Prof. Andreu Mas Colell
Consejaro de Economía y Conocimiento, Gobierno de Cataluña, Spain
28/02–02/03/2014
Impulsando la investigación.

Prof. Marijan Sunjic
University of Zagreb, Croatia
03/03–28/03/2014
Dynamical response and surface excitations in thin films.

Dr. Diego Peña Gil
Universidad de Santiago de Compostela, Spain
06/03–07/03/2014
Building nanographenes by organic synthesis in solution.

Dr. Emanuele Maggio
University of Warwick, Coventry, United Kingdom
06/03–07/03/2014
Theory of dye sensitised solar cells

Prof. John Inglesfield
University of Wales Cardiff, United Kingdom
07/03–04/04/2014
Embedding in photonics and plasmon bands in metallic nanostructures.

Dr. Kenta Kuroda
Hiroshima Jogakuin University, Hiroshima, Japan
15/03–19/03/2014
Photoemission measurements of electronic structure of topological insulators.

Prof. Akio Kimura
Hiroshima Jogakuin University, Hiroshima, Japan
16/03–19/03/2014
Photoemission measurements of electronic structure of topological insulators.

Lucia Ortega Álvarez (PhD Student)
Instituto de Ciencia y Tecnología de Polímeros, CSIC, Madrid, Spain
20/03–21/03/2014
Synthesis and characterization of rubber nanocompounds with shape memory.

Dr. Geza Giedke
Max-Planck-Institut für Quantenoptik, Garching, Germany
26/03–29/03/2014
Quantum Information and Quantum Optics: Implementations of QIP in atomic and solid-state systems.

Prof. Gustav Bihlmayer
IFF-FZ, Forschungszentrum Jülich, Germany
07/04–10/04/2014
Magnetism in low dimensions: Overlayers, wires and atoms.

Dr. François Konschelle
Institute for Quantum Information,Physikzentrum, RWTH Aachen, Germany
14/04–15/04/2014
Transport equations for superconductors in the presence of spin interaction.

Prof. Jürg Osterwalder
University of Zurich, Switzerland
15/04–17/04/2014
Functionalities from corrugated hexagonal boron nitride monolayers.

Dr. Rodrigo Humberto Aguilera del Toro
UASLP, Universidad Autónoma San Luis Potosí, México
20/04–23/04/2014
Nanostructure materials.

Dr. Florian Eich
University of Missouri, Columbia, Missouri, USA
22/04–16/05/2014
Condensed matter physics

Prof. Nobuhiko Azuma
Nagaoka University of Technology, Nagaoka, Japan
30/04–30/04/2014
The molecular structure of ice grain boundaries and its role in the dynamics of polar ice sheets.

Prof. Markus Hennrich
Institute for Experimental Physics, University of Innsbruck, Austria
03/05–06/05/2014
Quantum optics and spectroscopy.

Prof. Valery Tyuterev
Tomsk State Pedagogical University, Tomsk, Russia
04/05–31/05/2014
Phonons and electron dynamics in solids.

Prof. José Angel Martin Gago
Centro de Física de Materiales de Madrid, ICMM-CSIC, Madrid, Spain
08/05–10/05/2014
Nanoscience for studying the cosmos.
(A ERC-synergy grant for interdisciplinary science).

Prof. Remi Carminati
Institut Langevin, ESPCI ParisTech, France
11/05–14/05/2014
Statistics of single molecule fluorescence lifetimes in random media.

Prof. Aristide Dogariu
CREOL, University of Central Florida, USA
11/05–14/05/2014
Optical Forces.

Prof. M. Verónica Ganduglia Pirovano
Instituto de Catálisis y Petroquímica, CSIC, Madrid, Spain
12/05–14/05/2014
Cerium oxide surfaces reducibility and catalytic function: the role of electron localization.
A theoretical perspective.

Prof. Luisa Bausa
Instituto de Ciencia de Materiales Nicolas Cabrera, Universidad Autónoma de Madrid, Spain
13/05–13/05/2014
Effects of the interaction between localized surface plasmons and rare-earth ion based solid-state gain media.

Prof. Georgios Floudas
University of Ioannina, Greece
19/05–22/05/2014
Physics of soft matter.

Guillaume Vasseur (PhD Student)
Institut Jean Lamour, Université de Lorraine-CNRS, France
19/05–19/05/2014
One dimensional pi-conjugated band dispersion in polymeric chains.

Prof. Michaela Zimmermann
Max Planck Intitut, International Division Society, Münich, Germany
20/05–21/05/2014
Scientific communication, Max-Planck-Gesellschaft, Measures for international cooperation

Dr. Dietrich Foerster
CPMOH/LOMA Université de Bordeaux, France
20/05–21/05/2014, 28/05–29/05/2014
Test of new decomposition of Bloch's orbital products.

Dr. Saber Guedidda
IPCMS - Département Magnétisme des Objets NanoStructurés (DMONS), Strasbourg, France
20/05–21/05/2014
Molécules donneur-accepteur auto-assemblées pour la conversion photovoltaïque.

Prof. Kenneth S. Schweizer
University of Illinois at Urbana-Champaign, Illinois, USA
21/05–24/05/2014
Particle diffusion, topological entanglements and slow macromolecular dynamics in polymer nano-composites.

Prof. Frank Scheffold
Fribourg University, Switzerland
25/05–27/05/2014
Light scattering in colloidal suspensions and complex media.

Dr. Lorenzo Sponza
Institut des NanoSciences de Paris, INSP, France
28/05–29/05/2014
Damping, satellites and multiple excitations in oxides and nanostructures: effcient theoretical and numerical approaches towards a dynamical many-body theory.

Dr. Deung-Jang Choi
Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
29/05–01/06/2014
Composite magnetic systems created by atom manipulation.

Prof. Pere Alemany Cahner
Universitat de Barcelona, Barcelona
09/06–15/06/2014
How do you measure the symmetry of a molecule?

Dr. Héctor Vázquez Melis
Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic
09/06–12/06/2014
Modelling single molecule circuits.

Prof. Vladimir Chaldyshev
Ioffe Physico-Technical Institute, St. Petersburg, Russia
24/06–06/07/2014
Plasmonic on base of GaAs materials

Dr. Jens Brede
Institute of Applied Physics and Interdisciplinary Nanoscience Center, Hamburg, Germany
25/06–27/06/2014, 05/10–17/10/2014
Long-range magnetic coupling between nanoscale organic-metal hybrids mediated by a nanoskyrmion lattice.

Prof. Francisco José Garcia Vidal
Facultad de Ciencias, Universidad Autónoma de Madrid, Spain
01/07–29/07/2014
Plasmonics.

Dr. Francesca Balleto
King's College London, United Kingdom
01/07–01/07/2014
Unravelling morphologies and chemical ordering at the nanoscale.

Prof. Jorge E. Hirsch
Universidad de California, San Diego, California, USA
03/07–07/07/2014
Dynamic Hubbard model, high temperature superconductivity and the Meissner effect.

Dr. Marco Bernabei
Universidad de Barcelona
06/07–08/07/2014
Structure and dynamics of ring polymers.

Marina K Kuimova (PhD Student)
Imperial College London, UK
11/07–11/07/2014
Mapping microscopic viscosity using molecular rotors

Romain Dupuis (PhD Student)
CEMES/CNRS, Toulouse, France
16/07–18/07/2014
Cements and nanoadditions.

Prof. Pablo Ordejón Rontomé
Centre d'Investigació en Nanociència i Nanotecnologia (CSIC-ICN), Bellaterra, Barcelona, Spain
17/07–20/07/2014
Electronic transport in chemically modified and in amorphous graphite

Prof. Otto Muskens
University of Southampton, United Kingdom
22/07–25/07/2014
Plasmonic with novel material

Prof. Stefan Maier
Imperial College London, United Kingdom
23/07–27/07/2014
Plasmonics for sensing.

Dr. Mathieu Juan
University Macquarie, Sydney, Australia
23/07–25/07/2014
Optical forces: a link between classical and quantum mechanics.



Prof. Ulrich Höfer
Philipps-Universität Marburg, Germany
24/07/201423/08/2014, 07/11–08/11/2014
Resonance hopping on surfaces of simple metals.

Alessandro Romito (PhD Student)
Freie Universität Berlin, Germany
04/08/201406/08/2014
A scattering matrix topological index for interacting fermions in one-dimensional superconductors.

Dr. Javier Gorosabel Urkia
Instituto de Astrofísica de Andalucía, CSIC, Granada, Spain
04/08/201406/08/2014
Astronomical instrumentation: a window of opportunities.

Antonio Garcia Garcia (PhD Student)
University of Cambridge, United Kingdom and IFT, Universidade de Lisboa, Portugal
06/08–08/08/2014
Enhancing bulk superconductivity by engineering granular materials.

Prof. Ortwin Hess
Imperial College London, United Kingdom
17/08–21/08/2014
Nanophotonics in gain media.

Prof. Jochen Feldman
Lehrstuhl für Photonik und Optoelektronik, Ludwig-Maximilians-Universtität München, München, Germany
18/08–23/08/2014
Nanoplasmonics.

Dr. Luca Chirolli
Instituto de Ciencia de Materiales de Madrid CSIC-Madrid, Spain
21/08–24/08/2014
Transport properties of graphene.

Prof. Teunis Klapwijk
University of Delft, Holland
23/08–30/08/2014
Non-equilibrium properties of superconducting nanohybrids.

Dr. Benjamin W. Heinrich
Institut für Experimentalphysik, Freie Universität Berlin, Germany
26/08–26/08/2014
Magnetism of molecules on metal and superconducting surfaces.

Dr. Ewa Golas
Universidad de Gdansk, Poland
03/09–06/09/2014
Computer simulations of bio-inspired soft nanoparticles.

Antonio Correia (PhD Student)
Phantoms Foundation, Madrid, Spain
05/09–12/09/2014
Development of research networks.

Prof. José Manuel Hermida Ramón
Universidad de Vigo
12/09–12/09/2014
A combined quantum chemical/statistical mechanical method to simulate solvated systems in ground and excite state.

Prof. Archie Howie
University of Cambridge, United Kingdom
16/09–30/09/2014
Theory of valence electron excitations by fast electrons.

Prof. Jorge Kohanoff
Queen's University Belfast, Ireland
16/09–21/09/2014
Electronic structure calculation and ab initio molecular dynamic.

Prof. Christian Klinke
Institute of Physical Chemistry, University of Hamburg, Germany
17/09–21/09/2014
Two-dimensional colloidal nanostructures: synthesis and electrical transport.

Dr. Johan Gustafson
Div. of Synchrotron Radiation Research, Lund University, Sweden
17/09–19/09/2014
Seeing is believing - Novel in situ techniques for studies of model catalysts.

Dr. Leonor Chico Gómez
Instituto de Ciencia de Materiales de Madrid (ICMM), Spain
18/09–26/09/2014
Electronic structure calculations in graphene.

Prof. Cagla Meral
Middle East Technical University, Ankara, Turkey
18/09–27/09/2014
Hydration water in cement like materials.

Nick Papior Andersen (PhD Student)
DTU Nanotech, Technical University of Denmark, Lyngby, Denmark
21/09–20/10/2014
Methodology and efficient implementation of quantum transport theory in the TranSIESTA code.

Dr. Andrea Donarini
Institute of Theoretical Physics, University of Regensburg, Germany
25/09–27/09/2014
Transport characteristics of complex interacting nano-junctions.

Prof. Magnus Paulsson
Linnaeus University, Kalmar, Sweden
25/09–27/09/2014
Theoretical description of electron transport in nanoscale junctions.

Prof. Claude Cohen-Tannoudji
Laboratoire Kastler Brossel, París, France
30/09–03/10/2014
The dressed atom approach for describing atom-photon interactions.

Prof. Juan Ignacio Cirac
Max-Planck-Institut für Quantenoptik, Garching, Germany
01/10–03/10/2014
Quantum physics and computation

Dr. Antonio Politano
Università degli Studi della Calabria, Trieste, Italy
05/10–31/10/2014
Adsorption, electronic properties and collective excitations (phonons, plasmons) in thin metal films and graphen.

Prof. Friedhelm Bechstedt
Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und –optik, Jena Germany
05/10–18/10/2014
Many body perturbation theory applied to novel 2D materials, optical and energy loss spectroscopy.

Prof. Annemarie Pucci
Ruprecht Karls University of Heidelberg, Germany
06/10–05/11/2014
Infrared spectroscopy.

Prof. Manuel Aguilar Benitez De Lugo
CIEMAT
13/10–16/10/2014
Fundamental physics on the international space station.

Dr. Holger L. Meyerheim
Max-Planck-Institut für. Mikrostrukturphysik, Halle, Germany
13/10–15/10/2014
Structure analysis of clean and adsorbate covered Bi2Se3 using x-ray diffraction and x-ray absorption spectroscopy.

Ariane Koek
CERN, Meyrin, Canton de Genève, Switzerland
14/10–16/10/2014
Artists' Research Programmes.

Prof. Luis Alvarez Gaumé
CERN, Geneva, Switzerland
14/10–16/10/2014
Deconstructing mass.

Prof. Norbert Kroo
Wigner Physics Research Center of the Hungarian Academy of Sciences, Budapest, Hungary
18/10–22/10/2014
Some surface plasmon assisted nonlinear anomalies in a gold film at room temperature.

Prof. Peter Racz
Wigner Physics Research Center of the Hungarian Academy of Sciences, Budapest, Hungary
18/10–21/10/2014
Plasmonics, notably plasmon condensation.

Prof. Dilgam Taghiyev
Institute of Catalysis and Inorganic Chemistry, Azerbaijan National Academy of Sciences, Baku, Azerbaijan
16/11–23/11/2014
Topological materials.

Dr. Magalí Lingenfelder
Max Planck-EPFL Laboratory for Molecular Nanoscience EPFL, Lausanne, Switzerland
27/11–28/11/2014
A molecular interactions? roadmap to 2D functional nanostructures.

Prof. Alexander Protogenov
Institute of Applied Physics of Russian Academy of Sciences, Nizhnii Novgorod, Russia
28/11–24/12/2014
Transport properties of 3D topological insulators.

Fernando Delgado (PhD Student)
CFM (Ikerbasque Fellow), Donostia-San Sebastián, Spain
04/12–04/12/2014
Physics of a few magnetic atoms adsorbed on a surface.

Prof. Peter Apell
Chalmers University of Technology, Goteborg, Sweden
08/12–13/12/2014
Optical response in nanostructures.

Prof. Albert Fert
Unité Mixte de Physique CNRS/Thales, Université Paris Sud, France
14/12–17/12/2014
Spin-orbitronics, a new direction for spintronics: magnetic skyrmions, spin-orbit effects in 2D electron gas at surfaces and interfaces.

## Ikerbasque Research Professors

### Prof. Vyacheslav Silkin
Ultrafast dynamics of the one-particle and collective electronic excitations in metals and their surfaces. The study of electronic excitations at adsorbates on metal surfaces.

### Prof. Eugene Krasovskii
Electronic structure of nanosystems, surfaces and interfaces. Attosecond time resolved 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. Andrey Kazanskiy
Investigation of subfemto atto second processes in gases and solids caused by ultrashort laser pulses. Investigation of dynamics of electrons in suface and image states of noble metal and their interaction with adsorbates.

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

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

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

### Prof. Juan José Saenz Gutierrez
Ikerbasque Visiting Professor
Universidad Autónoma de Madrid, Spain
01/09/2013–31/08/2014
Nanophotonics. Modeling scanning probe microscopies.

### Prof. Geza Giedke
Quantum Information and Quantum Optics: Implementations of QIP in atomic and solid-state systems.

### Prof. Davide Donadio
Theory of nanostructures and transport.

## Ikerbasque Research Fellows

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

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

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

# Seminars

21/01/2014
Optical forces produced by localized sources.
Dr. Iñigo Liberal Olleta
Universidad Pública de Navarra, Pamplona, Spain

21/01/2014
Optical forces produced by localized sources.
Prof. Iñigo Ederra Urzainqui
Universidad Pública de Navarra, Pamplona, Spain

24/01/2014
Quantum transport in defected carbon-nanotubes.
Dr. Dario Bercioux
Dahlem Center for Complex Quantum Systems, Freie Universitaet Berlin, Germany

30/01/2014
Recent developments in black holes physics and astrophysics.
Prof. Jean-Pierre Luminet
Observatoire de Paris, LUTH, Meudon, France

06/02/2014
Interaction effects in magnetoplasmonics nanodisks.
Prof. Gaspar Armelles
Instituto de Microelectrónica de Madrid. IMM (CNM-CSIC), Madrid, Spain

18/02/2014
Towards a comprehensive model of surface enhanced raman scattering (SERS).
Prof. Andreas Otto
Universität Düsseldorf, Germany

28/02/2014
Impulsando la investigación.
Prof. Andreu Mas Colell
Consejaro de Economía y Conocimiento, Gobierno de Cataluña, Spain

07/03/2014
Building nanographenes by organic synthesis in solution.
Dr. Diego Peña Gil
Universidad de Santiago de Compostela, Spain

28/03/2014
Spins in quantum dots: quantum information and open systems dynamics.
Dr. Geza Giedke
Max-Planck-Institut für Quantenoptik, Garching, Germany

16/04/2014
Functionalities from corrugated hexagonal boron nitride monolayers.
Prof. Jürg Osterwalder
University of Zurich, Switzerland

30/04/2014
The molecular structure of ice grain boundaries and its role in the dynamics of polar ice sheets.
Prof. Nobuhiko Azuma
Nagaoka University of Technology, Nagaoka, Japan

09/05/2014
Nanoscience for studying the cosmos.
Prof. José Angel Martin Gago
Centro de Física de Materiales de Madrid, ICMM-CSIC, Madrid, Spain

13/05/2014
Cerium oxide surfaces reducibility and catalytic function: the role of electron localization? A theoretical perspective.
Prof. M. Verónica Ganduglia Pirovano
Instituto de Catálisis y Petroquímica, CSIC, Madrid

14.13/05/2014
Effects of the interaction between localized surface plasmons and rare-earth ion based solid-state gain media.
Prof. Luisa Bausa
Instituto de Ciencia de Materiales Nicolas Cabrera, Universidad Autónoma de Madrid, Spain

15.16/05/2014
Spin-charge conversion in interfacial electron liquids.
Prof. Giovanni Vignale
University of Missouri, Columbia, USA

16.19/05/2014
One dimensional pi-conjugated band dispersion in polymeric chains.
Guillaume Vasseur
Institut Jean Lamour, Université de Lorraine-CNRS, France

17.21/05/2014
Discotic liquid crystals of nanographenes. Self-assembly and molecular dynamics.
Prof. Georgios Floudas
University of Ioannina, Greece



21/05/2014
Max-Planck-Gesellschaft: Measures for international cooperation.
Prof. Michaela Zimmermann
Max Planck Intitut, International Division Society, Münich, Germany

22/05/2014
Unified theory of activated relaxation in molecular and polymeric liquids over 14 decades in time.
Prof. Kenneth S. Schweizer
University of Illinois, Urbana, USA

23/05/2014
Particle diffusion, topological entanglements and slow macromolecular dynamics in polymer nano-composites.
Prof. Kenneth S. Schweizer
University of Illinois, Urbana, USA

30/05/2014
Composite magnetic systems created by atom manipulation.
Dr. Deung-Jang Choi
Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

06/06/2014
Real-time electron dynamics with correlated wavefunction methods.
Prof. Peter Saalfrank
Institut für Chemie, Universität Postdam, Postdam-Golm, Germany

10/06/2014
Modelling single molecule circuits.
Dr. Héctor Vázquez Melis
Institute of Physics, Academy of Sciences of the Czech Republic, Praga, Czech Republic

12/06/2014
How do you measure the symmetry of a molecule?
Prof. Pere Alemany Cahner
Universitat de Barcelona, Spain

27/06/2014
Long-range magnetic coupling between nanoscale organic-metal hybrids mediated by a nanoskyrmion lattice.
Dr. Jens Brede
Institute of Applied Physics and Interdisciplinary Nanoscience Center Hamburg, Germany

01/07/2014
Unravelling morphologies and chemical ordering at the nanoscale.
Dr. Francesca Balleto
King's College London, United Kingdom

04/07/2014
Dynamic Hubbard model, high temperature superconductivity and the Meissner effect.
Prof. Jorge E. Hirsch
University of California, San Diego, USA

07/07/2014
Reliable energy and charge distribuion behavior of molecular and nanoscopic electronic states.
Prof. Luis Alberto Montero Cabrera
Facultad de Química, Universidad de la Habana, Cuba

11/07/2014
Mapping microscopic viscosity using molecular rotors.
Dr. Marina K Kuimova
Imperial College London, United Kingdom

17/07/2014
Realistic calculations of the isotopic fractionation factors of Si and Li for equilibriums involving liquid phases.
Romain Dupuis
CEMES/CNRS, Toulouse, France

18/07/2014
Electronic transport in chemically modified and in amorphous graphite.
Prof. Pablo Ordejón Rontomé
Centre d'Investigació en Nanociència i Nanotecnologia (CSIC-ICN), Bellaterra, Barcelona, Spain

23/07/2014
Optical forces: a link between classical and quantum mechanics.
Dr. Mathieu Juan
University Macquarie, Sidney, Australia

29/07/2014
Some aspects of spintronics in two-dimensional materials.
Dr. Miguel Angel Cazalilla
National University Singapore

30/07/2014
Have primordial gravitational waves been detected by BICEP2?
Prof. Jon Marcaide Osoro
Universidad de Valencia, Burjassot, Spain

07/08/2014
Enhancing bulk superconductivity by engineering granular materials.
Dr. Antonio Garcia Garcia
University of Cambridge, United Kingdom and IFT, Universidade de Lisboa, Portugal

21/08/2014
Nanoplasmonics meets Bio.
Prof. Jochen Feldman
Lehrstuhl für Photonik und Optoelektronik, Ludwig-Maximilians-Universtität München, Germany

26/08/2014
Magnetism of molecules on metal and superconducting surfaces.
Dr. Benjamin W. Heinrich
Institut für Experimentalphysik, Freie Universität, Berlin, Germany



12/09/2014
A combined quantum chemical/statistical mechanical method to simulate solvated systems in ground and excite state.
Prof. José Manuel Hermida Ramón
Universidad de Vigo, Spain

18/09/2014
Two-dimensional colloidal nanostructures: synthesis and electrical transport.
Prof. Christian Klinke
Institute of Physical Chemistry, University of Hamburg, Germany

18/09/2014
Seeing is believing - Novel in situ techniques for studies of model catalysts.
Dr. Johan Gustafson
Synchrotron Radiation Research, Lund University, Sweden

13/10/2014
Silicene and other honeycomb crystals from first principles.
Prof. Friedhelm Bechstedt
Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und –optik, Jena Germany

13/10/2014
Structure analysis of clean and adsorbate covered $Bi_2Se_3$ using x-ray diffraction and x-ray absorption spectroscopy.
Dr. Holger L. Meyerheim
Max-Planck-Institut für. Mikrostrukturphysik, Halle, Germany

14/10/2014
Fundamental physics on the international space station.
Prof. Manuel Aguilar Benitez De Lugo
CIEMAT, Madrid, Spain

14/10/2014
Deconstructing mass.
Prof. Luis Alvarez Gaumé
CERN, Geneve, Switzerland

15/10/2014
Colliding words - creative collisions between arts and science.
Ariane Koek
CERN, Meyrin, Canton de Genève, Switzerland

20/10/2014
Some surface plasmon assisted nonlinear anomalies in a gold film at room temperature.
Prof. Norbert Kroo
Wigner Physics Research Center of the Hungarian Academy of Sciences, Budapest, Hungary

29/10/2014
Surface science and plasmonics with infrared light.
Prof. Annemarie Pucci
Ruprecht Karls University of Heidelberg, Germany

27/11/2014
A molecular interactions? Roadmap to 2D functional nanostructures.
Dr. Magalí Lingenfelder
Max Planck-EPFL Laboratory for Molecular Nanoscience EPFL, Lausanne, Switzerland

04/12/2014
Physics of a few magnetic atoms adsorbed on a surface.
Fernando Delgado
CFM, Donostia-San Sebastián, Spain

05/12/2014
Are polarization and Magnetization Really Bulk Properties?
Prof. Raffaele Resta
Università di Trieste, Trieste, Italy

16/12/2014
Spin-orbitronics, a new direction for spintronics: magnetic skyrmions, spin-orbit effects in 2D electron gas at surfaces and interfaces.
Prof. Albert Fert
Unité Mixte de Physique CNRS/Thales, France





## 5th International Workshop on Photoluminescence in Rare Earths (PRE'14): Photonic Materials and Devices

May 13-16, 2014
Palacio Miramar, Donostia-San Sebastián, Spain

ORGANIZERS
Joaquin Fernandez (UPV/EHU, Spain)
Rolindes Balda (UPV/EHU, Spain)

This series of workshops started in 2005, It provides a forum for material scientists, chemists and physicists to discuss state of the art photonic materials based on rare earth ions. Both fundamental photoluminescence properties and application oriented material investigations are considered. Our main topics are:
Fundamental photoluminescence properties and spectroscopic measurements
Modelling, first-principles calculations, etc.
Photonic devices exploiting rare-earths characteristics
Rare-earth-doped crystalline materials
Transparent ceramics and glass-ceramic materials
Rare-earth optical amplifiers for telecommunication
Fiber lasers and micro-chip lasers
Phosphor materials for Solid-state Lighting
Downconvertors for photovoltaic applications
Rare-earth-doped materials for biological applications

*cont.*

CONTRIBUTIONS

Takunori Taira (Institute for Molecular Science, Japan)
RE3+ Ceramic Lasers for Energy: from Engine to Fusion Ignitions

John Ballato (Clemson University, USA)
Novel Rare-earth Doped Optical Fibers with Intrinsically Low Brillouin and Raman Gain

Patrice Camy (University of Caen, France)
Fluoride crystals for short pulse lasers and amplifiers

Luis Carlos (University of Aveiro, Portugal)
Nanoscale Thermometry with Rare Earths

Alicia Durán (Instituto de Cerámica y Vidrio, CSIC, Spain)
Transparent nano-glass ceramics doped with RE

Yasufumi Fujiwara (Osaka University, Japan)
Effects of impurity codoping on luminescence properties in Eu-doped GaN

Malgorzata Guzik (University of Wroclaw, Poland)
Rare earth-doped tungstates-based optical materials of cubic structure

Dariusz Hreniak (Polish academy of Sciences, Wroclaw, Poland)
Spectroscopic properties of Eu-doped pentaphosphate nanoceramics for white light-emitting devices

Daniel Jaque (Universidad Autónoma de Madrid, Spain)
Rare earth doped nanoparticles for infrared in vivo imaging and therapy

Tony Kenyon (University College London, United Kingdom)
Perspectives on Nanoclusters sensitization of erbium luminescence

Jorge Méndez Ramos (Universidad de La Laguna, Spain)
Rare-earth doped up-conversion materials for enhancing photocatalytic activity of water-splitting semiconductor electrodes

Markus Pollnau (University of Twente, Netherlands)
Rare-earth-ion-doped dielectric waveguides: Fabrication, spectroscopy, amplification, and lasing

Edwin Pun (City University of Hong Kong, Hong Kong China)
Rare earth doped superbroadband glass materials

Lothar Wondraczek (Otto-Schott-Institute, University of Jena, Germany)
Phosphors for light conversion in photosynthetic and photochemical energy harvesting

Ka-Leung Wong (Hong Kong Baptist University, Hong Kong China
Luminescence lanthanide materials for imaging of key cell cycle regulators and inhibition of cancer cells



# Trends in (Nano)Photonics 2014

July 24-24, 2014
Donostia International Physics Center, Donostia-San Sebastián, Spain

ORGANIZERS
Javier Aizpurua (CFM, CSIC-UPV/EHU, Spain)
Rubén Esteban (DIPC, Spain)

A one-day workshop devoted to the latest trends and findings by experts in Photonics and Nanophotonics from all over the world and collaborators in Donostia.

CONTRIBUTIONS

Francisco J. García Vidal (University Autónoma of Madrid, Spain)
Plasmonanoquanta: Transformation optics, quantum and non-linear phenomena in plasmonics

Otto Muskens (University of Southampton, United Kingdom)
Ultrafast nano-optics with plasmonic nanoantennas and silicon waveguides

Luis Liz-Marzán (biomaGUNE, Donostia-San Sebastián, Spain)
Metal nanoparticles with unusual morphologies

Paolo Vavassori (nanoGUNE, Donostia-San Sebastián, Spain)
Magnetoplasmonic nanoantenna metasurfaces for sensing and active control of light polarization

Juan José Sáenz (University Autónoma of Madrid and DIPC, Donostia-San Sebastián, Spain)
Intensity fluctuations produced by fluorescent emitters in complex media

Rainer Hillenbrand (nanoGUNE, Donostia-San Sebastián, Spain)
Infrared nanoimaging and nanospectroscopy

Yury Rakovich (CFM and UPV/EHU, Donostia-San Sebastián, Spain)
Optical effects in hybrid system of J-aggregates and plasmonic nanostructures

Andrey Borissov (Institute of molecular Sciences in Orsay, France)
Plasmon resonances in bimetallic nanoshells: quest for quantum effects

Scott Carney (University of Urbana, Illinois, USA)
Synthetic optical holography for probe microscopy

Stefan Maier (Imperial College London, United Kingdom)
Plasmonics for novel imaging, ultrafast lasing and compact directional emission

## Light in a hole: Workshop on confining light and molecules

August 18-19, 2014
Donostia International Physics Center, Donostia-San Sebastián, Spain

ORGANIZERS
Javier Aizpurua (CFM, CSIC-UPV/EHU, Spain)

In this workshop, four groups meet at DIPC to discuss ongoing collaborations in the field of optoelectronic networks formed by organometallic nanostructures as a platform to develop enhanced and selective SERS, catalysis, active optical control of modal response, and analyse particle on a mirror configurations, among others. The workshop is a unique oportunity to define the priorities and the roadmap of the recently awarded joint project led from Cambridge aiming at controlling and using the confinement of light and molecules in the presence of active and gain media.

PARTICIPANTS
Prof. Jeremy Baumberg (University of Cambridge, United Kingdom) with 6 participants
Prof. Oren Scherman (University of Cambridge, United Kingdom) with 3 participants
Prof. Ortwin Hess (Imperial College London, United Kingdom) with 1 participant
Prof. Javier Aizpurua (DIPC, Donostia-San Sebastián, Spain) with 3 participants

## Fuerzas y Túnel 2014

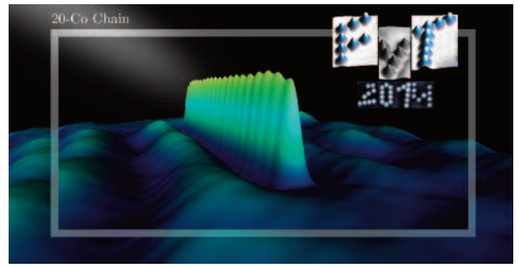
August 27-29, 2014
Palacio Miramar, Donostia-San Sebastián, Spain

ORGANIZERS
Celia Rogero Blanco (Centro de Física de Materiales (CSIC-UPV/EHU), Materials Physics Center (CFM), Donostia-San Sebastián, Spain)
Fernando Moreno-Herrero (Centro Nacional de Biotecnología (CNB-CSIC), Madrid, Spain)

Every two years the Spanish community working on scanning probe techniques meet for Fuerzas y Túnel (FyT). These biennial conferences began in Barcelona in 1998 and continued in Santiago de Compostela (2000), Zamora (2002), Vic (2004), Murcia (2006), Segovia (2008), Tarragona (2010), San Lorenzo de El Escorial (2012) and now in Donostia-San Sebastián. It brings together scientists who share an interest in applications, use, development and theoretical description of technology based in scanning probes. Sessions are dedicated to atomic force microscopy, scanning tunneling microscopy and theory of local probes techniques covering a wide range of applications from soft matter physics and biophysics to surface science in vacuum.

Most importantly, in this 9th edition, we honor Prof. Arturo M. Baró who will retire on 2014. Prof. Baró is one of the pioneers of SPM in Spain and one of our most renowned AFM/STM specialist abroad.

The Conference is included in the program of the XXXIII edition of "Cursos de Verano" of the University of Basque Country.




2014 FyT SPM Image Contest Winner: 20-Co Chain
Created by: Maria Moro (Instituto de Nanociencia de Aragón, Zaragoza, Spain)

STM image of a chain made by twenty Co atoms on a Ag(111) surface. The atomic chain was assembled along the [1-1 0] closed packed direction of the surface, by means of lateral manipulation technique. The distance between the Co atoms forming the chain is d=0.578 nm, two atomic distances of the Ag(111) lattice parameter, a=0.289 nm. The Fuerzas y Túnel 2014 logo was built by fifty seven Co atoms arranged with the STM tip by means of lateral manipulation technique on a Ag(111) surface. In this case, the distance between the Co atoms is three atomic distances, d=0.867 nm.

SCIENTIFIC COMMITTEE
Andrés Arnau (UPV/EHU)
Agustina Asenjo (ICMM)
Jaime Colchero (UM)
Jordi Fraxedas (CIN2)
José Miguel García (IMM)
Ricardo García (ICMM)
Julio Gómez (UAM)
José María Gómez-Rodríguez (UAM)
Amadeo López de Parga (UAM)
José Angel Martin-Gago (ICMM)
Javier Méndez (ICMM)
Aitor Mugarza (ICN)
Pedro J. de Pablo(UAM)
Jose Ignacio Pascual (CIC-Nanogune)
Rubén Pérez (UAM)
Roberto Otero (UAM)
Juan José Saenz (UAM)

For PhD students and postdocs presenting posters, there were two additional prizes sponsored by Bihurcrystal.

## 3rd Baskrete Industry Open Days

September 16-17, 2014
CEI Euskampus, UPV/EHU, DIPC, Tecnalia, CFM, CIC nanoGUNE, Donostia-San Sebastián, Spain

ORGANIZERS
XXX

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

# GDRi 2014

September 28 - October 1, 2014
Donostia International Physics Center, Donostia-San Sebastián, Spain

ORGANIZERS
Roland Pellenq (MIT, CNRS)
Emanuela Delgado (ETH Zurich)
Pierre Levitz (CNRS)
Jorge Sanchez-Dolado (TECNALIA)
Andres Ayuela (DIPC, CFM-CSIC)
Hegoi Manzano (UPV/EHU)
Sivina Cerveny (CFM-CSIC)

Workshop on Multiscale Porous Materials:

• Materials cover cements, clays, soils, porous glasses, porous ceramics including nuclear fuels...

• Models bridge time and length scales including texture measurement/simulation at different scales, mechanics (including fracture) at different scales, transport properties at different scales, long term behavior such as creep at different scales,...

The idea of setting-up the Groupement de Recherche International Multi-scale Materials Under the Nanoscope (GDRI, M2UN), is structuring the Physics, Chemistry, Mechanics and Materials Science communities on a common ground for developing an integrated approach (combining both simulation and experiments) for the prediction of texture properties from angstroms to micron and their evolution in time from nanoseconds to years of complex multi-scale materials such as clays (soil), cement, nuclear solid fuels, steels and ceramics. The M2UN GDRI is an initiative organized under the auspices of CNRS (www.cnrs.fr). This international research organization aims at promoting:

• Scientific exchanges through recurrent meetings collaborations between the different teams involved including visits of PhD students, post-doctoral associates and faculty.

• Educational activities and the spread of knowledge through the organizations of a thematic school, the Marseille Winter School on Multicale Porous Materials for Energy and Environment (2nd Edition, Jan 16-22, 2014, Aix-Marseille Polytech-ESIL, Luminy campus, Marseille).

• A platform from which participants can design grant proposals toward the US-NSF, the ESF and others funding agencies the emergence of a new field of research at the frontier between Science and Engineering.

The ambition of such a GDRI is formulating a conceptual tool named as the "nanoscope" that combines most advanced statistical Physics numerical simulations (such as accelerated Molecular Dynamics) and experiments (such as X-Ray tomography and microscopy...). This "nanoscope" tools aims at elucidating the 3D texture of those multi-scale (and most of the time porous) materials from the scale of atoms to microns focusing in particular of mechanical and transport properties. The coupling between numerical simulation and experiments is a major theme of the GDRI and is one of the most challenging issues in Material Science, Mechanics and condensed matter Physics. From a computational point of view, two ways are usually put forward: a utopian one that aims at developing "the ultimate simulation code" and a more pragmatic one that considers associating different scales by passing the "right" piece of information to the scale above and create an interface, for instance between atomistic description and finite element methods that are operational at the scale of microns and above. We have obviously chosen this second approach. We aim at spanning not only length by also time scales and address phenomena such visco-elastic deformations and creep that cover many length and time scale. To achieve this, important experimental developments are needed to observe and understand materials texture and transport properties at different scales; these range from X-ray microcopy and tomography, electron microscopy, nano-indentation, dispersive wave spectroscopy, NMR-relaxometry. The scientific project of the GDRI M2UN is both fundamental and applied as it merges Science and Engineering in a single research field: as physicists or Material scientists are driven by engineering challenges and engineers move into the fundamentals of physics, a shift of paradigm is taking place that enables progress at the interface of physics and engineering for a large variety of critical problems that are at the core of many society, environmental and economy concerns in connection with durability and sustainability issues in construction, transportation, energy and waste management.

## CONTRIBUTIONS

**Session 1: Textures and Mechanics**
Chair: Pierre Levitz

Enrico Masoero
C-S-H at the Mesoscale: Structure and Water Sorption

Franz-Joseph Ulm
Fracture Toughness of Multi-scale Materials.

Emanuela Del Gado
Early stages of cement hydration and mesco-scale texture of C-S-H

Rainer Hillebrannd
Nano-FTIR in minerals

Henri Van Damme
Urban Physics, City Texture Matters

Benoit Coasne
Multi-Scale Modeling of Molecular Transport in Shales

**Session 2: Experimental Characterization of Confinement**
Chairs: Emanuela Del Gado, Silvina Cerveny

Jean-Pierre Korb, Benjamin Nicot, Aline Louis-Joseph, Salvatore Bubici, Gianni Ferrante
Dynamics and Wettability of Oil and Water in Oil Shales

Jan Swenson
What can we learn about bulk water from dielectric relaxation studies of confined water and aqueous solutions?

Heloisa N. Bordallo
Neutron scattering, a powerful tool to study water in confinement

Michael Vogel
NMR study of the dynamics of confined water

Session 3: Nano-Micro Mechanics
Chair: Franz J. Ulm

Guillaume Galliero, Hai Hoang
Fluids confined in slit nanopores: from local transport properties to shear induced swelling

Gilles Pijaudier-Cabot, Laurent Perrier, David Grégoire
Enhanced poromechanics for the modeling of swelling in microporous materials:
Coupled effects, size effects and upscaling issues

Jeremy Berthonneau, Christian Hoover, Olivier Grauby, Alain Baronnet, Roland Pellenq, Franz-Joseph Ulm
Experimental nano-chemo-mechanial testing on minerals: from elasticity to fracture

David N. Espinoza, Matthieu Vandamme, Jean-Michel Pereira, Patrick Dangla,Sandrine Vidal-Gilbert
Experimental characterization, modeling, and impact on permeability, of adsorption-deformation couplings in coal samples in presence of $CO_2$

Eduardo Duque-Redondo, Hegoi Manzano, Nerea Epelde, Virginia Martínez-Martínez, Iñigo López-Arbeloa
Input from Molecular Modelling for the Design of Hybrid Photoactive Materials

David Grégoire, Fadi Khaddour, Gilles Pijaudier-Cabot
Upscaling Poiseuille's and Knudsen's flows to predict gas permeability in damaged porous media

Hegoi Manzano
Hydration of Mineral Surfaces: new insight from reactive force field Molecular Dynamics

Session 4: Fluid under Confinement
Chair: Jose S. Dolado

Carine Malheiro, Frédéric Plantier, Bruno Mendiboure, Christelle Miqueu
Use of Density Functional Theory for the modeling of adsorption of methane, water and their binary mixture in slit micropores.

Qianqian Wang, Yanhua Guo, Xiaodong Shen, Feng Li, Hegoi Manzano, Iñigo López-Arbeloa
Water adsorption and dissociation on the β-C2S (100) cement clinker surface from first-principles calculations

Houria Chemmi, Dominique Petit, Renaud Denoyel, Jean-Pierre Korb, Pierre Levitz
Confinement impact on the dynamics of water in calibrated mesoporous silica

Mohammad.-Javad, Abdolhosseini Qomi, Roland Pellenq
Nanoscale Dynamics of water in CSH



Jean-Mathieu Vanson
Simulation of adsorption and transport in hierarchical porous materials using Lattice-Boltzmann model

P. Levitz, C. Bousige, B. Coasne
Potentiality of the pore network topological graphs to analyze structure and dynamics of complex porous media: focus on cement paste and disordered carbon membranes

Session 5: Carbon Materials
Chair: Andrés Ayuela

Roland Pellenq
The Journal of Nano and Micromechanics, ASCE

Julio A. Alonso, Iván Cabria, María J. López
Doped Nanoporous Carbons for Hydrogen Storage.

Matthieu Salanne, Clarisse Péan, Céline Merlet, Benjamin Rotenberg, Paul Madden, Barbara Daffos, Pierre-Louis Taberna, Patrice Simon, Yury Gogotsi
Modeling Ion Adsorption and Dynamics in Nanoporous Carbon Electrodes

Julien Colell, Guillaume Galliero
Molecular Simulation of Fluid Distribution and Transport Properties in Shales Organic Matter

Gyorgy Hantal, Laurent Brochard, Roland J.M. Pellenq, Franz J. Ulm, Benoit Coasne
Mechanical behavior and failure of clay-organic composites: overall toughening upon interface weakening? Numerical simulations and theory

## XI International Ontology Congress

October 1-4, 2014
University of the Basque Country and Chillida Leku Museum, Donostia-San Sebastian, Spain
October 6-7, 2014
Universitat Autònoma de Barcelona, Spain
October 23, 2014
Fundación Paideia, A Coruña, Spain

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

International Scientific Committee
A. Aspect (Paris); P. Aubenque (Paris) F.J. Ayala (California); J. Bouveresse (Paris); †E. Chillida (San Sebastián); A. Grünbaum (Pittsburgh); †W. Lamb (Arizona); T. Marco (Madrid); U. Moulines (München); †I. Prigogine (Brussels); H. Putnam (Boston). Coordinator: V. Gómez Pin (Barcelona)

Organizing Committee
Gotzon Arrizabalaga (UPV/EHU); José Ignacio Galparsoro (UPV/EHU); Juan Ramón Makuso; Gemma Cortel (UAB); Andreu Ballús (UAB). Coordinator: Victor Gómez Pin (UAB).

Under the Honorary Presidency of Bas van Fraassen
OLD QUESTIONS ON PHYSIS, CONTEMPORARY APPROACHES
I. The Problem of Realism: State of The Art (Under the patronage of DIPC)
  1. San Sebastián
  2. Barcelona - 50 Years of Bell`s Theorem: Physics and Reality
II. THE RISE OF THE HUMAN ANIMAL (Under the Patronage of ATAPUERCA)

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David Albert (Columbia University, New York, USA)
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Steven French (University of Leeds, United Kingdom)
Tim Maudlin (New York University, USA)
James Ladyman (University of Bristol, United Kingdom)
Andrés Moya (President of the SSBE)
Jean-Michel Raimond (École Normale Supérieure, PAris, France)
Simon Saunders (University of Oxford, United Kingdom)
Mauricio Suarez (Universidad Complutense de Madrid, Spain)
Bas Van Fraassen (Princeton University, New Jersey, USA)



## Mestizajes Workshop 2014
## (II Encuentro sobre Literatura y Ciencia)

November 18-19, 2014
CFM, Donostia-San Sebastian, Spain

ORGANIZER
Gustavo Ariel Schwartz (CFM-CSIC and DIPC)

Mestizajes constituye un espacio alternativo para el encuentro de artistas, científicos y humanistas. Un lugar para el debate, para pensar diferente, para imaginar; un lugar para la búsqueda, para el encuentro y también para el desacuerdo; un lugar para la generación y la divulgación de nuevas formas de conocimiento. Mestizajes pretende abrir un camino que permita transitar la frontera entre arte y ciencia y crear allí un terreno fértil para la generación de nuevas ideas. Mediante workshops, conferencias, residencias y colaboraciones, Mestizajes pretende fomentar la participación activa y una mirada crítica de la realidad desde una perspectiva innovadora y vanguardista. La idea fundacional de Mestizajes es que se ha abierto una grieta en la muralla que separa arte y ciencia y que es posible transitar esa frontera e internarnos en un territorio emergente cargado de un enorme potencial humano e intelectual.

Razón, Intuición e Imaginación
Los objetivos principales de Mestizajes son favorecer el diálogo entre ciencias, artes y humanidades; fomentar la diversidad intelectual y promover el mestizaje entre distintas formas de conocimiento; analizar el surgimiento simultáneo de ideas en diversos campos del conocimiento, como así también estimular la influencia recíproca, entre las ciencias, las artes y las humanidades. Mestizajes se propone como un espacio para romper con la hiper-especialización del conocimiento y desde donde promover el multilingüismo cognitivo. Mestizajes pretende contribuir a la construcción de un conocimiento más amplio donde arte, ciencia y humanidades se complementen y se enriquezcan mutuamente.

En esta ocasión, el tema de debate se centrará en torno a la Razón, la Intuición y la Imaginación en la Literatura y en la Ciencia. Nos proponemos explorar la intuición literaria y su relación con la neurociencia, la génesis metafórica de los conceptos científicos, la construcción del mundo desde la literatura y desde la ciencia y las relaciones entre razón e intuición.

Temas del encuentro: Matemática, intuición e imaginario colectivo, Intuición literaria y neurociencia, Razón, intuición e imaginación en ciencia y en literatura, La construcción del mundo desde la literatura y la ciencia

PARTICIPANTES
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Presentación

Gustavo A. Schwartz (CSIC-CFM and DIPC, Donostia-San Sebastián)
Apertura

Jorge Wagensberg (Facultad de Física – Universidad de Barcelona)
Sobre el talento y el talante interdisciplinario

Amelia Gamoneda (Facultad de Filología – Universidad de Salamanca)
¿Cómo sabe una metáfora? Poética y ciencia

Moderador: Gustavo A. Schwartz (CSIC-CFM and DIPC, Donostia-San Sebastián)
Discusión – Mesa redonda Jorge Wagensberg / Amelia Gamoneda

Itziar Laka (Facultad de Letras, UPV/EHU, Vitoria
Intuición, arte y lenguaje

# Higher Education

DIPC School

## International Summer School on Semiconductor Interfaces – Methods and Model Systems

July 27-31, 2014
Palacio de Miramar, Donostia-San Sebatián, Spain

ORGANIZERS
Dr. Daniel Sánchez Portal (Centro de Física de Materiales CSIC-UPV/EHU and DIPC, Donostia-San Sebatián, Spain)
Prof. Krestin Volz (Philipps-Universität Marburg, Germany)

Interfaces between solids play a decisive role in modern material sciences and their technological applications. Among the most prominent examples are semiconductor devices, which have been miniaturized to such an extent that their optical and electronic properties are determined decisively by internal interfaces. Other relevant examples are interfaces in solar cells, the separation between carriers of opposite signs taking place there, and the organic/inorganic interfaces of functionalized particles and surfaces in biosensors.

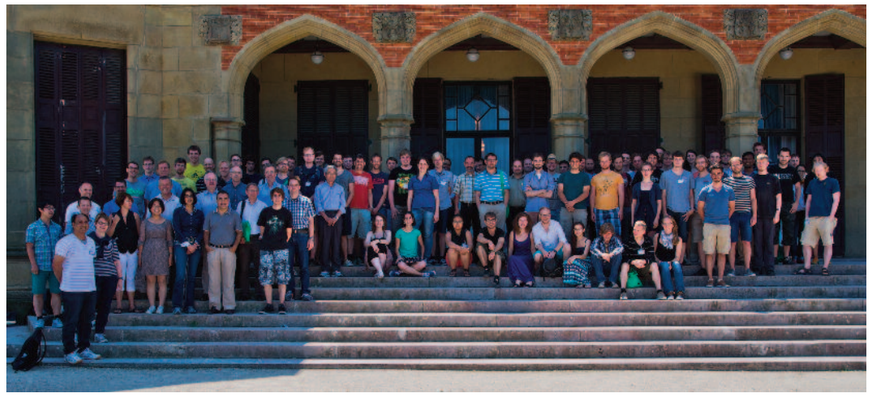
This summer school is motivated by to this growing interest in the study of buried interfaces and aims to present the latest experimental and theoretical developments in the field. The school is aimed at a postgraduate level. We will have three speakers/subtopics every day covering different aspects of the subject. The speakers are internationally leading experts in their respective field. Every speaker gives two lectures. A tutorial-like introduction to the state-of-the art in her/his field (60+20 min) followed by a talk covering her/his own latest work (30+10 min).

*cont.*

Some of the subjects covered in the course:
Scanning transmission electron microscopy, laser and time-resolved optical and photoemission spectroscopies, characterization of interfaces using synchrotron and FEL-based X-Ray spectroscopy, semiconductor heteroepitaxy, epitaxial growth of growth organic model interface, surface functionalization with organic molecules, ab initio calculations of organic/inorganic interfaces.

Institutional support and funding:
The course is organized within the Summer Courses of the University of the Basque Country and is held at the Palacio de Miramar in Donostia-San Sebastián. The institutions that support the event are:

- University of the Basque Country UPV/EHU
- Collaborative Research Center on Structure and Dynamics of Internal Interfaces (SFB 1083) and Research Training Group "Functionalization of Semiconductors", Philipps-Universität Marburg, Germany
- Centro de Física de Materiales de San Sebastián, CFM UPV/EHU-CSIC, Donostia-San Sebastián, Spain
- Donostia International Physics Center (DIPC), Donostia-San Sebastián, Spain



DIPC School

## Frontiers of Condensed Matter

August 25 – September 4, 2014
Donostia-San Sebastián, Spain

This DIPC School aims at offering Master and PhD students a training program in the area of Condensed Matter Physics. It is organized jointly by the Materials Physics Center CFM-CSIC (Spain), Ecole Doctorale de Physique de Grenoble (France), the Casimir Research School Delft-Leiden (Netherlands), and the Ecole Doctorale de Physique et d`Astrophysique (PHAST), Lyon (France).

The courses are complemented by more specialized research seminars on timely topics.

During the school, there is plenty of time for informal discussions between participants and lecturers. A poster session is organized. The school can host 60 participants, (including lecturers - limited by the size of the lecture hall), and is intended for experimentalists and theoreticians.

LECTURERS AND TOPICS
L. Di Carlo (TU Delft) Quantum Information
A. Levy Yeyati (Universidad Autónoma de Madrid) Superconducting point-contacts
J. Meyer (U. Grenoble) Topological Phases
Y. Nazarov (TU Delft) Quantum Transport
F. Pistolesi (U. Bordeaux) Nanomechanics
J. Zaanen (U. Leiden) Strongly-correlated Systems

SEMINARS SPEAKERS
J. Aizpurua (CFM, San Sebastian)
S. Bergeret (CFM, San Sebastian)
P. Brouwer (Freie Universität Berlin)
F. Hekking (U. Grenoble)
T. Klapwijk (TU Delft)
L. Kouwenhoven (TU Delft)
T. Meunier (U. Grenoble)
I. Pascual (Nanogune)
J. Van Ruitenbeek (U. Leiden)
V. Vitelli (U. Leiden)

ORGANIZING COMMITTEE
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Frank Hekking (U. Grenoble)
Julia Meyer (U. Grenoble)
Sebastian Bergeret (CFM-DIPC)
Francisco López Gejo (CFM)

*cont.*

CONTRIBUTIONS

J. Zaanen (U. Leiden)
Quantum criticality: from high Tc superconductivity to black holes. (I)

T. Klapwijk (TU Delft)
Direct observation of ballistic Andreev-reflection: an overview

S. Bergeret (CSIC-DIPC)
Introduction to Superconductor-Ferromagnet Nanohybrids

J. Zaanen (U. Leiden)
Quantum criticality: from high Tc superconductivity to black holes. (II)

F. Pistolesi (CNRS)
Introduction to Nano-ElectroMechanical Systems (I)

T. Meunier (U. Grenoble)
Quantum spin manipulation and spin transfer of a single electron

F. Pistolesi (CNRS)
Introduction to Nano-ElectroMechanical Systems (II)

J. Zaanen (U. Leiden)
Quantum criticality: from high Tc superconductivity to black holes. (III)

L. Di Carlo (TU Delft)
Quantum Information (I)

J. Aizpurua (CSIC-DIPC)
Nanophotonics with plasmons

P. Brouwer (Freie U. Berlin)
Majorana Wires

L. Di Carlo (TU Delft)
Quantum Information (III)

J. Van Ruitenbeek (U. Leiden)
Single molecules as electronic devices

Y. Nazarov (TU Delft)
- Scattering approach to quantum transport (I)

J. Meyer (U. Grenoble)
Topological Phases (I)

V. Vitelli (U. Leiden)
Topological Mechanics

N. Hussey (HFML)
Contrasting criticalities in the cuprates and pnictides

J. Meyer (U. Grenoble)
Topological Phases (II)

Y. Nazarov (TU Delft)
Scattering approach to quantum transport (II)

A. Levy Yeyati (UAM)
The Hamiltonian approach to quantum transport in nanostructures (I)

I. Pascual (CIC nanoGune)
Tunnel spectroscopy of atoms and molecules: exciting electrons, spins and vibrations

Y. Nazarov (TU Delft)
Scattering approach to quantum transport (III)

J. Meyer (U. Grenoble)
Topological Phases (III)

A. Levy Yeyati (UAM)
The Hamiltonian approach to quantum transport in nanostructures (II)

Y. Nazarov (TU Delft)
Scattering approach to quantum transport (II)

L. Kouwenhoven (TU Delft)
Experimental detection of Majoranas

A. Levy Yeyati (UAM)
The Hamiltonian approach to quantum transport in nanostructures (III)

DIPC School

## Scanning Probe Microscopy: A Tribute to Heinrich Rohrer

September 5-12, 2014
Donostia-San Sebastián, Spain

This DIPC School is a tribute to Heinrich Rohrer (1933-2013) who shared the 1986 Nobel Prize in Physics with Gerd Binnig for the design of the scanning tunneling microscope (STM). This invention gave scientists the ability to image, measure and manipulate atoms for the first time.

The lectures cover basic concepts and fundamentals of different SPM techniques including STM, Near Field Optical Microscopy (SNOM) and Atomic (AFM), Electrostatic (EFM) or Magnetic Force microscopes (MFM). It also discusses advanced topics such as time resolved SPM, density functional theoretical approaches, single molecule SPM or biology and nano-medicine applications.

The main topics are complemented with a workshop and seminars on state-of-the-art SPM research, with the participation of some of the most relevant scientists who will give a first-person view of latest discoveries in this field.

ORGANIZERS
Andrés Arnau (CFM-CSIC-EHU)
Ricardo Díez-Muiño (DIPC, CFM-CSIC-EHU)
Rainer Hillenbrand (NanoGune)
Enrique Ortega (CFM-CSIC-EHU)
Jose Ignacio Pascual (CIC nanoGune)
Juan José Sáenz (DIPC, Ikerbasque; IFIMAC-UAM)

Course

## Field Theoretical Methods in Solid State Physics

March 10, 14, 17, 21 and 24, 2014
DIPC, Donostia-San Sebastián, Spain

PROFESSOR
Marijan Sunjic (University of Zagreb, Croatia)

Prof. Sunjic is a well-known specialist in condensed matter theory and has worked extensively in the fields of photoemission and electronic excitations. We invited him to prepare a course that could be delivered to young researchers and he kindly agreed to design a program on field theoretical methods in solid state physics. It should be of particular interest to master students, PhD students and post-docs but it is open to anyone interested in the topic.

March 10, 2014
**Quantum mechanical description of many-body systems**
Many body systems, nonseparability of Schroedinger equation: exact and approximate methods; many-body wave functions – bosons and fermions. Second quantization: Creation, annihilation and field operators, physical states and observables.

March 14, 2014
**Green's functions - propagators. Single-particle function - definitions, properties.**
Spectral function. Free particle Green's function; boson Green's function. Perturbation expansion of the Green's function, Wick's theorem, lowest order terms; Feynman diagrams and their evaluation.

March 17, 2014
**Some applications of Green's function method**
Vacuum fluctuations, connected and disconnected diagrams. Linked Cluster Theorem. Reducible and irreducible diagrams. Particle self-energy, Dyson equation. Quasiparticle - definition and properties.

March 21, 2014
**Ground state energy**
Coulomb (Hartree) and exchange (Fock) energies, correlation energy. Boson Green's functions, Fermion-boson (electron-phonon) interaction. Polaron, renormalization of particle mass and energy.

March 24, 2014
**Linear response theory**
Correlation functions and the differential cross section. Dynamical and static structure factors. Neutron and x-ray scattering in crystals: differential cross section, elastic scattering, Debye-Waller factor, phonon emission and absorption.

## Theses

Structure and electronics of donor-acceptor blends.
**Elisabeth Goiri Little**
February 2014
Supervisors: Dimas G. de Oteyza and Enrique Ortega

Elastic and inelastic electron transport through alkane-based molecular junctions.
**Giuseppe Foti**
September 2014
Supervisors: Thomas Frederiksen and Andres Arnau

## Master's Degree Program

# UPV/EHU Research Master's in Nanoscience

DIPC collaborates in the official postgraduate program in nanoscience organized by the Materials Physics Department of the University of the Basque Country (UPV/EHU) and the Center of Materials Physics (CSIC-UPV/EHU) "Master's in Nanoscience".

The Research Master's in Nanoscience has been offered since 2007 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.

In addition, DIPC plays a valuable role, providing essential infrastructure and funding, within its means, to help ensure the proper development of the program.



## Credits

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