DIPC

Donostia International Physics Center

Activity Report

10/11

On the cover

DIPC Activity Report 2010/11

A new twist

According to computer simulations, atoms in solid helium can flow without friction when arranged in a regular, spiral structure.

Cover image credit: Leibniz-Institut für Kristallzüchtung (Germany)

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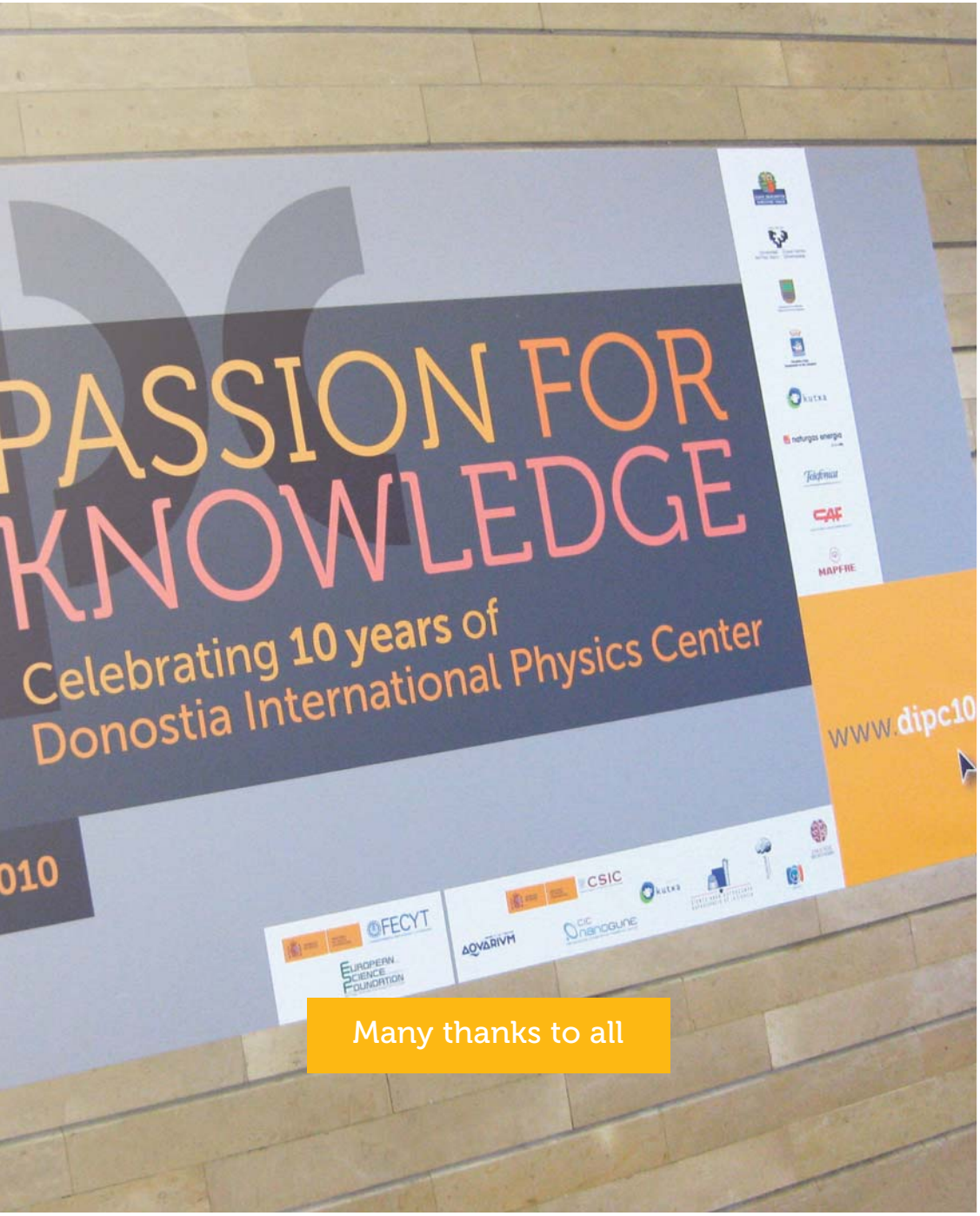
DIPC Activity Report 2010/11

Pedro Miguel Echenique, President of DIPC, opens **Passion for Knowledge** with an introduction to keynote speakers, Robert Langer and Aaron Ciechanover.

> Since its very conception DIPC has stood for the promotion of high quality science. This tall order demands a platform in which ideas are freely exchanged, new objectives are set and shared, and new personal bonds are established; a space in which the enthusiasm for discovery reigns over bureaucracy, convention and routine.

The DIPC concept envisages gathering scientists from the University of the Basque Country (UPV/EHU) or the Materials Physics Center (CSIC-UPV/EHU), with visiting scientists from around the world in a boundless consortium: The DIPC Community.

Recently, DIPC has actively participated in securing the ranking as Campus of International Excellence (CIE) for the Euskampus project. The Euskampus CIE is a project led by UPV/EHU, in alliance with DIPC and TECNALIA, for the development of new projects on education, research, innovation and internationalization with its sights set on becoming a driving force in achieving improved competitiveness and socioeconomic growth of the Basque Country. DIPC is also a Founding Partner of the Euskampus Foundation, constituted to guarantee the governance and continuity of the CIE Euskampus Project.



The status of a center in the international scientific community depends on the impact of the work it publishes. The higher the impact, the greater the international exposure, and hence the louring effect on world-class visiting researchers and students.

DIPC is a center devoted to research at the cutting-edge of science, but DIPC also assumes the responsibility of conveying scientific knowledge to society. We believe that scientific culture contributes to the progress and freedom of society.

The center offers meeting spaces for scientists and organizes events that bring science to the citizen. We strive to generate an intellectual climate intended to awaken curiosity, interest, fascination and enthusiasm for knowledge, especially among the young. The DIPC Science Communication Program has helped achieve these objectives. In 2010, we celebrated our first decade by organizing Passion for Knowledge, a festival of activities for the scientific community and the general public all around the city of Donostia-San Sebastián, running from April to November. The format chosen for Passion for Knowledge was groundbreaking. The event was designed as a festival of knowledge with three major sections: The Lectures, to communicate science, The City, to raise the presence of science in the city itself —both of which were open to anyone wishing to attend—, and The Workshops, reserved for the scientific community. Passion for Knowledge proved a resounding success, not just because of the extraordinary quality of the invited speakers, but above all, because of the breathtaking response of the public. We are delighted and proud for the shared success of Passion for Knowledge in bringing scientists and citizens together.

I would like to finish by thanking the Board of Trustees, the staff and all the DIPC research associates for a job well done.

Pedro Miguel Echenique

Board of Trustees

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Research Activity for 2010 and 2011

Research

434
scientific **articles**
1628 since 2000

31,183
citations since 2000
(Approximation as of May 2012)

2010-2011

405
visiting **researchers**
1568 since 2000

97
seminars
529 since 2000

Seminars

Workshops

19
workshops
70 since 2000

	2000	01	02	03	04	05	06	07	08	09	10	11
Publications	54	72	90	112	116	134	140	155	156	163	**213**	**223**
Seminars	17	34	51	44	47	46	53	45	49	46	**47**	**50**
Workshops	4	5	3	5	4	6	5	6	5	8	**14**	**5**
Visitors	24	58	111	115	103	123	145	197	103	184	**184**	**221**

Public Events

General Science Communication Program

The DIPC's Science Communication Program has the principal objective of helping to bring the contents and values of science and technology to society. This is a crucial activity in the design of activities of the DIPC.

The DIPC is a research center dedicated to research on the borders of scientific knowledge; it also assumes the responsibility of conveying to citizens this knowledge which, we believe, contributes to the progress, culture and freedom of society. The DIPC proposes meeting spaces for scientists and organizes contacts between science and society, cultivating an intellectual climate intended to awaken curiosity, interest, fascination and enthusiasm for knowledge. The DIPC Science Communication Program seeks to help establish a fluid, permanent dialogue between science and society, between scientists and citizens. The aim of the initiative is to foster responsible social and scientific progress in a free and tolerant intellectual environment showing science to be an accessible cultural activity attractive to all publics. The DIPC particularly wishes to cultivate a suitable climate for encouraging the youngest among us to study science and technology, thereby creating a dynamic reserve and channeling the talent of the coming generations.

In 2011, we pressed on in our commitment to bring science to society. We continued the Kutxa Lectures, looking at enormously interesting hot topics with top class researchers and excellent communicators; the Encounters between students and Nobel Laureates to continue awakening scientific vocations; and organized a new edition of the On Zientzia competition, maintaining our collaboration with the Elhuyar Foundation.

On December 2, 2011, we organized a conference on scientific communication attended, among others, by two winners of Nobel Prizes for Physics and a Prince of Asturias Award-winner. In the

morning, we once again turned our eyes towards secondary school students, potential future researchers, who had the opportunity to attend an Encounter. Forty-four schools from all over the Basque Country participated, with a total of 132 students and 44 teachers. In the afternoon, we held the event 'Frontiers of Science', open to the general public, the program of which featured brief talks on subjects like physics, bio-medicine or cosmology and a round table with the presence of the two Nobel Laureates, open to participation of the 250 people who filled the hall.

On-zientzia contest

Since 2010, a yearly contest to award the best amateur videos created to promote scientific outreach has been organized by DIPC in collaboration with Elhuyar Editorial, and the program Teknopolis from the Basque television (EITB). The success of the first edition in 2010 with more than 50 videos participating freely, generated the interest and joy to organize this event again in 2011. The reception of the videos participating in the present edition has been just closed in April 2012 with 48 videos.
http://www.onzientzia.tv/

Kutxa Lectures

These series of lectures open to the general public started in 2010, as part of Passion for Knowledge in collaboration with Kutxa Obra Social. The excellent feedback of the public and attendees encouraged us to continue organizing them. In 2011, we organized a session to explain the public a very hot topic at that moment, are the neutrinos faster than light? The speaker, Prof. Jose Ignacio La Torre, from the University of Barcelona, is an expert on the topic and a great communicator. The answer from the public was exceptional, with 250 attendees completing the capacity of the hall.
October 5, 2011. 'Neutrinos: Einstein seguramente tenía razón' by Jose Ignacio La Torre, Professor at the University of Barcelona
Andia Kutxa Hall. Donostia - San Sebastian

Seminars by Nobel Laureates

Very distinguished scientists have been invited to the DIPC to give a seminar or share their experiences in science and their views on different topics with the young (and not so young) researchers in an informal manner.
November 28, 2011. Prof. Sydney Brenner, Nobel Prize in Physiology or Medicine 2002, gave a seminar at the DIPC headquarters oriented to the local scientists from any field but open to the whole university community. 'Reading the Human Genome: the reconstruction of the Past'

Frontiers of Science

This open event was a kind of a special Kutxa Lessons. As we explained before, the program featured brief talks on subjects like physics, bio-medicine or cosmology by experts on the field, and a round table with the presence of the two Nobel Laureates.
December 2, 2011. Andia Kutxa Hall. Donostia - San Sebastian

Encounters

DIPC has organized every year since 2009 a set of Encounters between Nobel Laureates and secondary school students (about 12-14 years old) where the young students can chat and discuss about different issues of life, science and technological impact with eminent and prestigious Nobel Laureates. This experience has exceeded all the expectations regarding the incredible feedback given by school students as well as the joy experienced by the laureates when checking the vivid and lively interaction given by the young Basque students. There have been already three editions, where Nobel Laureates H. Kroto (2009), H. Rohrer (2009), J.M. Lehn (2010), F. Wilczek (2010), A. Yonath (2010), C. Cohen-Tannoudji (2011) and A. Fert (2011), as well as a Prince of Asturias Award-winner, J. I. Cirac (2011) and S. Earle (2010), have participated.

PASSION FOR KNOWLEDGE

Celebrating **10 years** of
Donostia International Physics Center



Welcome
Pedro Miguel Echenique and **Isabel Celaá**, Minister of the Department of Education, Universities and Research of the Basque Government

Opening Lectures

Robert Langer
2008 PRINCE OF ASTURIAS AWARD
Novel biomaterials

Aaron Ciechanover
2004 NOBEL PRIZE IN CHEMISTRY
Drug Development in the 21st century.
Are we going to cure all diseases?










Celebrating **10 years** · Celebrando **10 años** · **10 urteak** ospatzen

THE LECTURES

Juan Ignacio Cirac
2006 PRINCE OF ASTURIAS AWARD
Quantum Physics:
A new view of Nature
and much more

Jean-Marie Lehn
1987 NOBEL PRIZE IN CHEMISTRY
From matter to life:
Chemistry? Chemistry!

Richard Ernst
1991 NOBEL PRIZE IN CHEMISTRY
Passion and responsibility.
Education, magnetic resonance,
and Central Asian painting art

Sylvia Earle
2009 TED PRIZE
The urgency of exploring
the deep frontier

Dudley Herschbach
1986 NOBEL PRIZE IN CHEMISTRY
Taming wild molecules

Theodor Hänsch
2005 NOBEL PRIZE IN PHYSICS
A passion for precision

Frank Wilczek
2004 NOBEL PRIZE IN PHYSICS
Anticipating a new Golden Age

Bernardo Atxaga
2008 PREMIO LETTERARIO INTERNAZIONALE MONDELLO
Poem for my friend Lazkano

Roald Hoffmann
1981 NOBEL PRIZE IN CHEMISTRY
Chemistry's essential tensions:
Three views

Claude Cohen-Tannoudji
1997 NOBEL PRIZE IN PHYSICS
Using light for manipulating atoms

Luis De Pablo
2003 PRIX MUSICAL INTERNATIONAL ARTHUR HONEGGER
Passion for music:
another kind of "knowledge"

Sir John Pendry
FELLOW OF THE ROYAL SOCIETY
Invisible cloaks and a perfect lens

Ada Yonath
2009 NOBEL PRIZE IN CHEMISTRY
Everests, polar bears,
unpaved roads, antibiotics and
the evolving ribosome

Heinrich Rohrer
1986 NOBEL PRIZE IN PHYSICS
Science, fascination, passion

THE CITY

kutxa LECTURES

May 13 - June 17, 2010

Pedro Miguel Echenique Chairman
Juan Colmenero Vice-chairman
Alberto López Basaguren Vice-chairman

EXECUTIVE COMMITTEE
Igor Campillo Secretary General
Ricardo Díez Muiño Head of the The Workshops program
Unai Ugalde Head of the The Lectures program
Enrique Zárate Head of The City program

Throughout 2010, under the motto, City of science, Science in the city, a wide range of activities were organized in collaboration with other entities. Science, culture and leisure all converge in these activities, which were open to the general public. The Kutxa Lecture, given by local researchers, shared their experience in the world of research as well as giving an introduction to the topics to be presented at the main event in September.

CONTRIBUTIONS

Pedro Miguel Echenique
Passion for Knowledge: The sublime usefulness of useful science

Jose Maria Pitarke
From the large to the small: quasars, quarks, and the nanoscale

Fernando Cossio
Science, nature and art: chemistry and its metaphors

Javier Aizpurua
When light becomes small

Juan Colmenero
Molecule by Molecule: self-assembly and nanotechnology

THE CITY

PASSION FOR THE SEA

September 24-29, 2010

Pedro Miguel Echenique Chairman
Juan Colmenero Vice-chairman
Alberto López Basaguren Vice-chairman

EXECUTIVE COMMITTEE
Igor Campillo Secretary General
Ricardo Díez Muiño Head of the The Workshops program
Unai Ugalde Head of the The Lectures program
Enrique Zárate Head of The City program

Passion for knowledge is also passion for life, passion for nature and environment which, in a city like San Sebastian, necessarily entails a Passion for the Sea. In collaboration with the Aquarium Donostia-San Sebastian, a program of sea-related activities was designed with particular emphasis on the specific lines of research developed in the Aquarium. The Passion for the Sea lectures featured world-leading researchers, who are also regular collaborators with the Aquarium. The speakers spoke of some of the challenges they face in their current research activity.

CONTRIBUTIONS

Charles A. Farwell (Tune Research and Conservation Center, Hopkins Marine Station, Monterey Bay Aquarium, USA)
Bluefin tuna, one of the most advanced fish species in the ocean, an example of speed and endurance

Fernando de la Gándara (Marine farming plant, Spanish Oceanography Institute, Mazarrón, Spain)
Domestication of bluefin tuna: the lastest challenge of seawater culture

DOCUMENTARIES

September 24-29, 2010

A series of documentaries on nature and sealife was also shown at the Aquarium including some outstanding documentaries from the Submarine Cinema Festival and from other cinema contests on nature.

THE CITY

Biosanitary Environment ENCOUNTER

September 27, 2010

Pedro Miguel Echenique Chairman
Juan Colmenero Vice-chairman
Alberto López Basaguren Vice-chairman

EXECUTIVE COMMITTEE
Igor Campillo Secretary General
Ricardo Díez Muiño Head of the The Workshops program
Unai Ugalde Head of the The Lectures program
Enrique Zárate Head of The City program

Passion for Knowledge aimed to approach the biosanitary environment too, where science and investigation play such an important role. To do so, we held an encounter where Aaron Ciechanover, Richard Ernst, and Robert Langer shared their experiences with doctors, researchers and representatives of the biosciences and biosanitary environment.

Moderator: Pedro Miguel Echenique

Aaron Ciechanover 2004 Nobel Prize in Chemistry

Richard Ernst 1991 Nobel Prize in Chemistry

Robert Langer 2008 Prince of Asturias Award

THE CITY

kutxaEspacio ENCOUNTER for Students

September 28, 2010

Pedro Miguel Echenique Chairman
Juan Colmenero Vice-chairman
Alberto López Basaguren Vice-chairman

EXECUTIVE COMMITTEE
Igor Campillo Secretary General
Ricardo Díez Muiño Head of the The Workshops program
Unai Ugalde Head of the The Lectures program
Enrique Zárate Head of The City program

Juan Ignacio Cirac, Jean-Marie Lehn y Frank Wilczek Sylvia Earle and Ada Yonath encounter secondary science students and teachers. They spoke about their particular passion for knowledge and the students asked questions in regard to their work and experience in science.

Moderator: Pedro Miguel Echenique

Juan Ignacio Cirac 2006 Prince of Asturias Award

Jean-Marie Lehn 1987 Nobel Prize in Chemistry

Frank Wilczek 2004 Nobel Prize in Physics

THE CITY

kutxaEspacio ENCOUNTER for Teachers

September 29, 2010

Pedro Miguel Echenique Chairman
Juan Colmenero Vice-chairman
Alberto López Basaguren Vice-chairman

EXECUTIVE COMMITTEE
Igor Campillo Secretary General
Ricardo Díez Muiño Head of the The Workshops program
Unai Ugalde Head of the The Lectures program
Enrique Zárate Head of The City program

Claude Cohen-Tannoudji, Dudley Herschbach, and Heinrich Rohrer reflexed on the educational system in general and on issues related to teaching science and technology especially models and experiences from different countries, undervaluation of the teaching of science today, and motivating students and teachers.

Moderator: **Pedro Miguel Echenique**

Claude Cohen-Tannoudji 1997 Nobel Prize in Physics

Dudley Herschbach 1986 Nobel Prize in Chemistry

Heinrich Rohrer 1986 Nobel Prize in Physics

THE CITY

Aquarium ENCOUNTER for Students

September 30, 2010

Pedro Miguel Echenique Chairman
Juan Colmenero Vice-chairman
Alberto López Basaguren Vice-chairman

EXECUTIVE COMMITTEE
Igor Campillo Secretary General
Ricardo Díez Muiño Head of the The Workshops program
Unai Ugalde Head of the The Lectures program
Enrique Zárate Head of The City program

Sylvia Earle and Ada Yonath encounter secondary science students and teachers. They spoke about their particular passion for knowledge and the students asked questions in regard to their work and experience in science.

Moderator: **Pedro Miguel Echenique**

Sylvia Earle 2009 TED Prize

Ada Yonath 2009 Nobel Prize in Chemistry

THE CITY

PASSION FOR ART

September 20-October 10, 2010

Pedro Miguel Echenique Chairman
Juan Colmenero Vice-chairman
Alberto López Basaguren Vice-chairman

EXECUTIVE COMMITTEE
Igor Campillo Secretary General
Ricardo Díez Muiño Head of the The Workshops program
Unai Ugalde Head of the The Lectures program
Enrique Zárate Head of The City program

FOTCIENCIA

FOTCIENCIA is a scientific photography contest organised by the Higher Council of Scientific Research (CSIC) and the Spanish Foundation for Science and Technology (FECYT). The event takes science and technology closer to the public by presenting an artistic, aesthetic vision suggested by scientific images and written commentaries on the scientific facts being depicted.

The exhibition, comprising a selection of 50 photos selected by the jury, reached San Sebastian after being on show in many cities in Europe, Asia and America. FOTCIENCIA photos are a public resource for the dissemination of science.

NANOART21

NanoArt21 was founded by the scientist and artist Cris Orfescu, and is directed at promoting NanoArt throughout the world as a reflection on technological development. Orfescu considers that NanoArt is a more attractive and effective way of communicating with the general public in order to provide information on the new technologies of the 21st century. NanoArt aims to raise the awareness of the general public with regard to nanotechnology and its impact on our lives.

"NanoArt is a new art discipline at the art-science-technology intersections. It features nanolandscapes (molecular and atomic landscapes which are natural structures of matter at molecular and atomic scales) and nanosculptures (structures created by scientists and artists by manipulating matter at molecular and atomic scales using chemical and physical processes). These structures are visualized with powerful research tools like scanning electron microscopes and atomic force microscopes and their scientific images are captured and further processed by using different artistic techniques to convert them into artworks showcased for large audiences." (Cris Orfescu)

THE LECTURES

PASSION FOR KNOWLEDGE

September 27 - October 1, 2010

Pedro Miguel Echenique Chairman
Juan Colmenero Vice-chairman
Alberto López Basaguren Vice-chairman

EXECUTIVE COMMITTEE
Igor Campillo Secretary General
Ricardo Díez Muiño Head of the The Workshops program
Unai Ugalde Head of the The Lectures program
Enrique Zárate Head of The City program

ORGANIZING COMMITTEE
Fernando Cossío President, Fundación Ikerbasque
José María Mato General Director, CIC bioGUNE and biomaGune
Ginés Morata Professor of Research, Centro de Biología Molecular of CSIC-UAM
Luis Oro Director, Instituto Universitario de Catálisis Homogénea, University of Zaragoza
Rafael Pardo Director, Fundación BBVA
Jose Maria Pitarke General Director, CIC nanoGUNE
Joan Rodés Ex-general director, Hospital Clinic of Barcelona
Félix Yndurain Head of Department, Faculty of Sciences of the Universidad Autónoma of Madrid

The Lectures of Passion for Knowledge brought together speakers from different disciplines, cultures and thinking to engage the public with stories of personal exploration. Nobel laureates and world-leading experts will show their passion for knowledge and deep commitment to research. They spoke about the key moments, developments, challenges and implications of their research and works. The Lectures combined scientific rigor and entertainment to awake the curiosity, the interest, the enthusiasm and critical thinking of the public at large.

CONTRIBUTIONS

Bernando Atxaga **Poem for my friend Lazkano**
Aaron Ciechanover **Drug Development in the 21st century. Are we going to cure all diseases?**
Juan Ignacio Cirac **Quantum Physics: A new view of Nature and much more**
Claude Cohen-Tannoudji **Using light for manipulating atoms**
Luis De Pablo **Passion for music: another kind of "knowledge"**
Sylvia A. Earle **The urgency of exploring the deep frontier**
Richard Ernst **Passion and responsibility. Education, magnetic resonance, and Central Asian painting art**
Theodor Hänsch **A passion for precision**
Dudley Herschbach **Taming wild molecules**
Roald Hoffmann **Chemistry's essential tensions: Three views**
Robert Langer **Novel biomaterials**
Jean-Marie Lehn **From matter to life: Chemistry? Chemistry!**
Sir John Pendry **Invisible cloaks and a perfect lens**
Heinrich Rohrer **Science, fascination, passion**
Frank Wilczek **Anticipating a new Golden Age**
Ada Yonath **Everests, polar bears, unpaved roads, antibiotics and the evolving ribosome**

Scientific Highlights

2010

2011

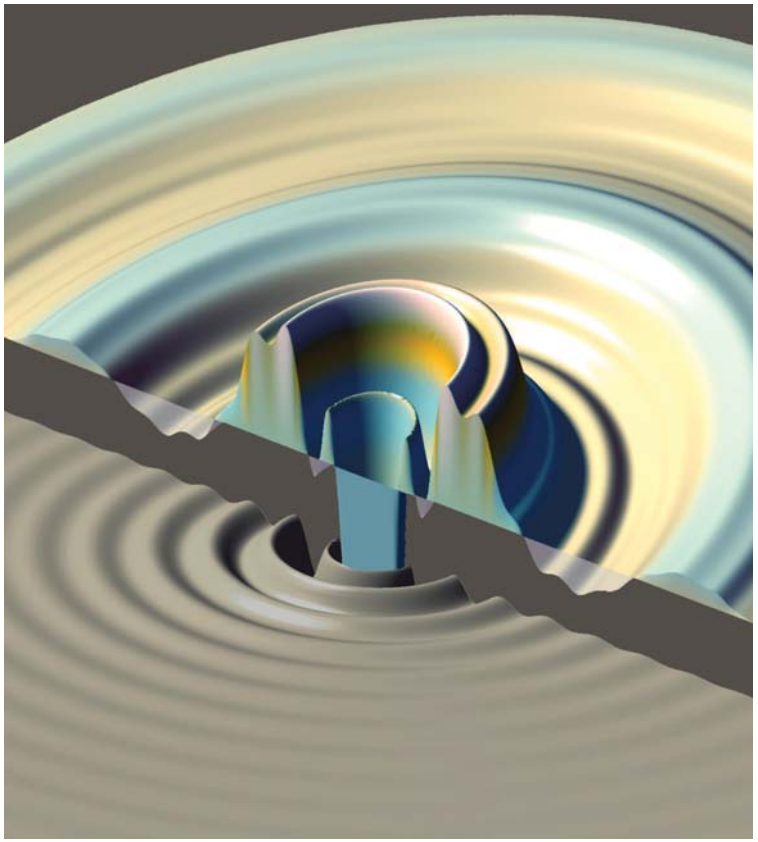
Acoustic surface plasmon on Cu(111)

K. Pohl, B. Diaconescu, G. Vercelli, L. Vattuone, V.M. Silkin, E.V. Chulkov, P.M. Echenique, M. Rocca
EPL 90, 57006 (2010)

An acoustic surface plasmon (ASP) is a novel collective electronic excitation at metal surfaces. This new mode has a linear (or acoustic-like) dispersion, i.e. it can be excited at very low energy and wavelength, allowing it to participate in many dynamical processes, such as chemical reactions and nano-sensors at surfaces and sub-wavelength optics and photonic devices as well as new microscopy techniques.

After the original discovery of an ASP on the close-packed surface of beryllium a joint experimental-theoretical study in collaboration with researchers at DIPC has shown that the ASP can also been excited and detected on Cu(111). Thus, it is evidence that the ASP is indeed a general phenomenon on metal surfaces that support a partially occupied surface state within a wide bulk energy gap. Non-local screening of the surface electrons due to bulk electrons creates the ASP.

Of particular interest is the interaction of the ASP with light: nm-size objects at surfaces, such as atomic steps or molecular structures, can provide coupling between light and ASPs of much lower wavelength than conventional surface plasmons. In this way, the new mode can serve as a tool to confine light in a broad frequency range up to optical frequencies on surface areas of a few nanometers, thus facilitating control of events at metal surfaces with both high spatial (nm) and high temporal (fs) resolution. Another consequence of the acoustic-like character of the ASP dispersion is that both phase and group velocities are the same, so signals can be transmitted undistorted along the surface. The theoretically estimated ASP decay lengths of 100 to 1,000 nm for medium (100 meV) to far (10 meV) infrared are an appealing prospect for the field of nano-optics.



Theoretically simulated electron surface wave patterns created by a point charge located close to a metal surface: The conventional Friedel oscillations (bottom) and a snapshot of the dynamical ASP wave (top) propagating from the center.

The acoustic surface plasmon is a general phenomenon on metal surfaces that support a partially occupied surface state within a wide bulk energy gap.

A versatile "click" chemistry precursor of functional polystyrene nanoparticles

L. Oria, R. Aguado, J.A. Pomposo, and J. Colmenero
Advanced Materials 22, 3038 (2010)

Highly efficient routes to well-defined single-chain nanoparticles with size below 10 nm are really scarce. Recently, we have reported the facile synthesis of a versatile "click" chemistry precursor of ultra-small polystyrene single-chain nanoparticles (size ≈4 nm).

Functional nanoparticles (NPs) are becoming important building blocks in the emerging fields of nanomedicine, nanolithography and nanoelectronics, among others. In recent years several unexpected nano-scale effects have been discovered for these new materials. However, useful synthetic routes to single-molecule polymeric NPs in the 2–15 nm size range are certainly scarce in spite of the enormous potential predicted for these materials. In this sense, the main requirements for a versatile synthetic route to single-chain cross-linked polymeric NPs are: i) easy incorporation of coupling precursors into the individual polymer chains, ii) highly efficient and selective cross-linking (coupling) reaction, and iii) appropriate room temperature reaction conditions favoring intramolecular coupling versus intermolecular cross-linking.

In recent years, exquisite control over the composition, molecular weight and molecular weight distribution of synthetic macromolecules (including block and random copolymers) has been achieved using (user-friendly) controlled/living radical polymerization techniques, such as reversible addition-fragmentation chain transfer (RAFT) polymerization. Additionally, "click" chemistry methodologies and specifically the copper-catalyzed cycloaddition of alkynes and azides (Figure 1) are currently being used in polymer and materials science for easy and almost quantitative functionalization of synthetic polymers, biomolecules and inorganic nanoparticles. In fact, the combination of RAFT polymerization and "click" chemistry meets all the above requirements for the synthesis of well-defined single-chain cross-linked polymeric NPs.

Recently, we have "*mise-a-point*" the synthesis of a new and versatile "click" chemistry precursor of functional polystyrene nanoparticles (PS-NPs) by the combination of RAFT copolymerization and a subsequent very efficient functionalization step. This procedure allows the preparation of the "clickable" nanoparticle-precursor starting from a simple styrene copolymer, opening the way to PS-NPs that could be potentially used as processing additives or fluorescent contrast agents, among other applications. As illustrated in Figure 2 (A), a significant viscosity drop was found in nanocomposites of neat natural rubber (cis-1,4-polyisoprene) and ultra-small functional PS-NPs at very low NP content. In fact, this is the first report of rubber nanocomposites with reduced melt viscosity arising from the presence of well-dispersed individual polymeric NPs. In addition, Figure 2 (B) demonstrates the useful fluorescence emission properties of ultra-small PS-NPs.

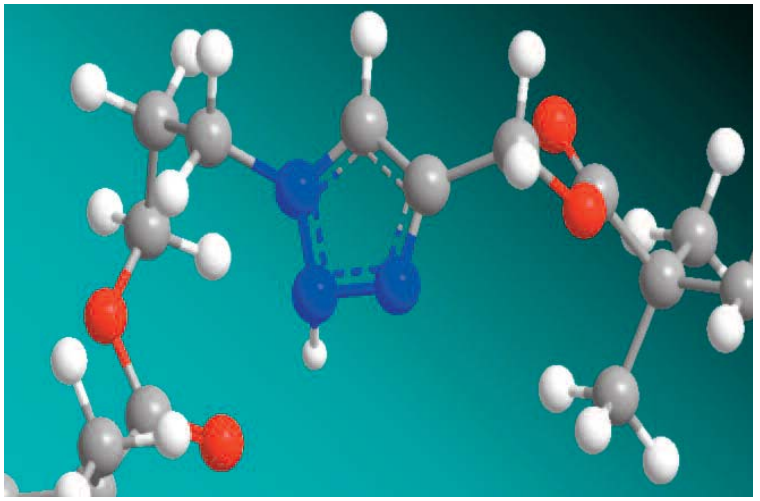


Figure 1. Illustration of the "click" chemisty concept: in the present of a copper-catalyst, azide group (blue color) reacts very fast with alkyne group (grey color) to give a triazole ring.

A versatile "click" chemistry precursor of ultra-small functional polystyrene nanoparticles (size ≈4 nm) has been synthesized.

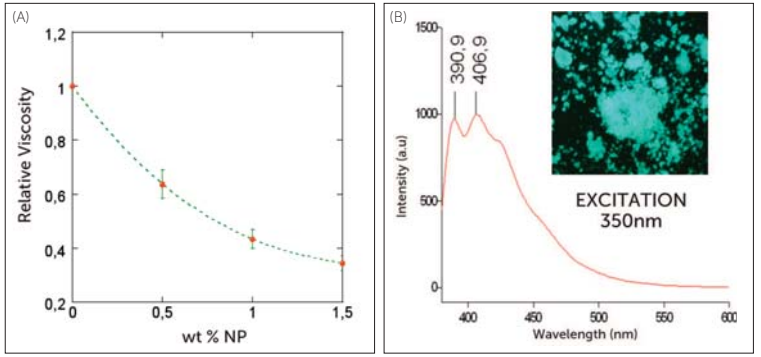


Figure 2. Illustration of the properties of ultra-small functional polystyrene nanoparticles (size ≈4 nm): (A) as processing additives, inducing a significant viscosity drop in neat natural rubber (cis-1,4-polyisoprene); (B) as fluorescent contrast agents, showing a strong fluorescence emission band with two clear peaks at 391 and 407 nm.

Sodium: a charge-transfer insulator at high pressures

M. Gatti, I. Tokatly, and A. Rubio
Physical Review Letters 104, 216404 (2010)

A simple metal under pressure? It becomes a complex insulator.

Sodium at ambient pressure is the simplest of the simple metals. But under pressure the situation changes dramatically. In fact, from a simple, uncorrelated, reflective metal, sodium turns into a complex, correlated, transparent insulator.

In this paper, we show by first-principles calculations that in the optical response of transparent sodium the electron-hole interaction is very important. It gives rise to the formation of an unusual kind of charge-transfer exciton that proceeds from the interstitial distribution of valence electrons repelled away from the ionic cores by the Coulomb interaction and the Pauli repulsion. In this sense, sodium behaves as an unconventional inorganic electride, characterised by the simplest possible anion: an electronic charge without ionic core. Moreover, the absorption spectrum shows a strong anisotropy with light polarization that just at pressures above the metal-insulator transition manifests as sodium being optically transparent in one direction, but reflecting light as a normal metal in the other. Our result also provides a fingerprint for the crystal structure of dense sodium.

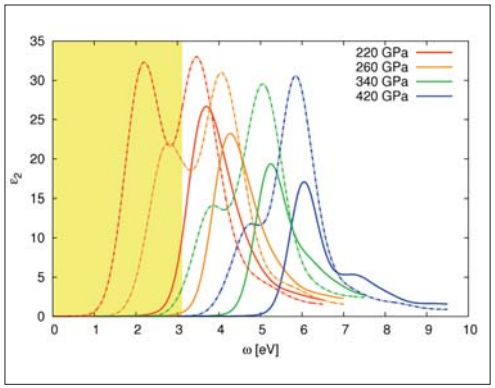


Figure 1. Polarization dependence of the transparency. Yellow zone: energy range of visible light (up to 3.1 eV). At low pressures Na is transparent in the in-plane direction (solid lines) and reflective along c axis (dot-dashed lines). By increasing pressure, the peak in the in-plane direction (solid lines) is quite rigidly blueshifted and its intensity is reduced accordingly (as an effect of the f-sum rule). Instead, for the polarization along the c axis (dot-dashed lines) at low pressures the spectrum is characterised by a double peak, while by increasing pressure the first peak progressively looses strength developing as a shoulder of the second one.

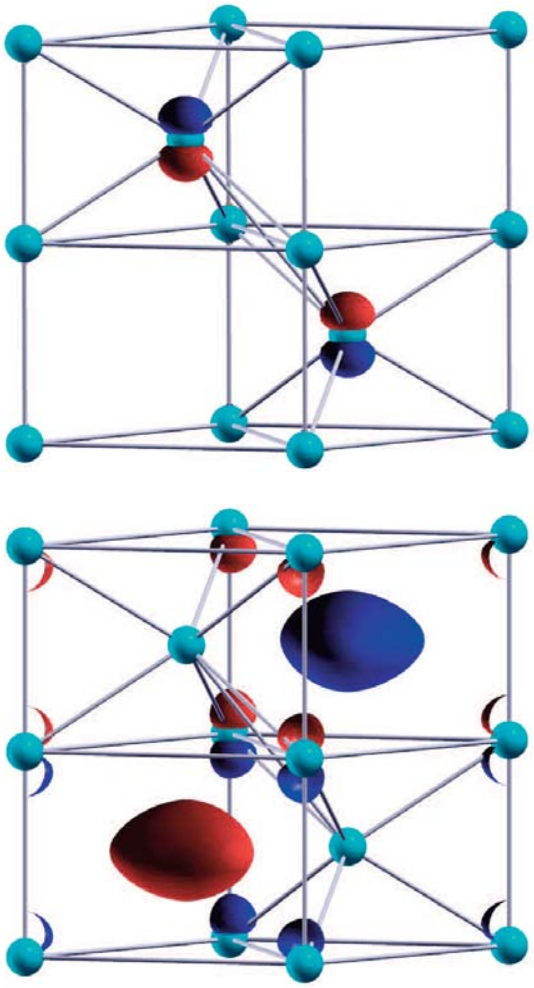


Figure 2. Electronic charge distribution involved in the lowest-energy charge-transfer excitation: by absorbing light, the electronic charge moves from the situation in the bottom panel to the situation in the upper panel.

Optical spectroscopy of conductive molecular junctions in plasmonic cavities

O. Perez-Gonzalez, N. Zabala, A.G. Borisov, N.J. Halas, P. Nordlander, and J. Aizpurua
Nano Letters 10, 3090 (2010)

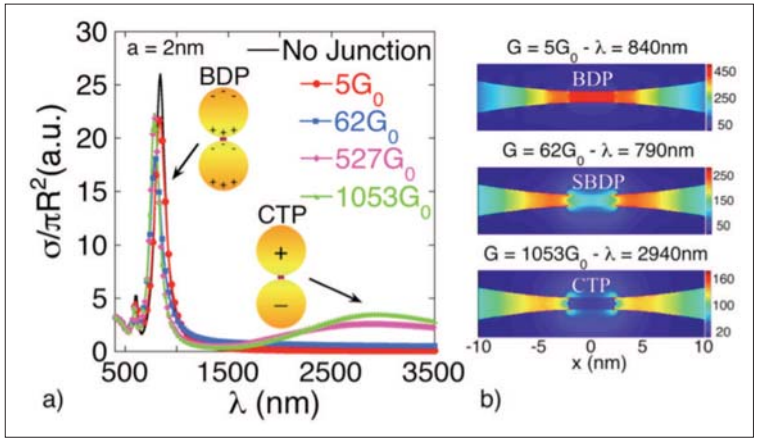
In the last decade fundamental advances have been achieved in the fields of molecular electronics and plasmonics. In particular, the optical properties of adjacent nanoparticle pairs have been explained using exact numerical calculations of Maxwell equations and hybridization models. Recent simultaneous measurements of electronic conduction and Raman spectroscopy in molecular junctions have suggested the possibility of sensing individual molecules connecting both optical and transport properties in the junctions.

Here we present a theoretical study of this connection between molecular electronics and plasmonics in a system composed of a conductive molecular junction bridging a plasmonic cavity. The model system consists of a conductive bridge linking two gold nanoshells. The nanoshells are formed by a silica core surrounded by a gold shell and the molecular junction is modelled as a cylinder of radius a linking both nanoshells. The conductivity of the junction, σ, is related to its conductance, G, through the geometrical parameters of the system. Therefore, for a given size of the linker, we modify the conductivity of the junction varying the number n of quanta of conductance, nG_0 ($G_0 \equiv 2e^2/h \cong 77.5mS$). Maxwell's equations are solved via a boundary element method (BEM) to obtain the electromagnetic fields and the optical extinction spectra.

Two different regimes can be identified in the optical response (see figure). For the short wavelength regime, we first notice a broadening of the plasmon resonance as conductance is increased, followed by a slight blue-shift until a saturation point is reached. Then, the resonance becomes narrower again as conductance continues to be increased but its wavelength remains unaltered. This plasmon resonant mode is denoted as the Bonding Dimer Plasmon (BDP). For the long wavelength regime, there is no appreciable change when conductance takes small values. However, for very large values of conductance, a new highly red-shifted resonance emerges. This resonance is the Charge Transfer Plasmon (CTP) and its main feature is its tunability.

A simple resistor model is used to explain both the initial decrease of the optical extinction intensity of the BDP and its progressive recovery for further increase of the conductance. It is also possible to notice a slight blue-shift which corresponds to a screened Coulomb interaction at the junction between the gold shells. Moreover, a threshold value of the conductance can be identified. This threshold value denotes the conductance where the optical properties of the junction start being affected by the transport properties. A good estimation for the threshold conductance can be obtained by relating the time of flight of the electrons involved in the transport process with the time of the optical cycle of the plasmonic resonances of the cavity.

The study of this kind of spectral changes in plasmonic cavities might serve as a probe of molecular conductance and transport processes in the visible part of the spectrum, a range which is not accessible through electrical measurements.



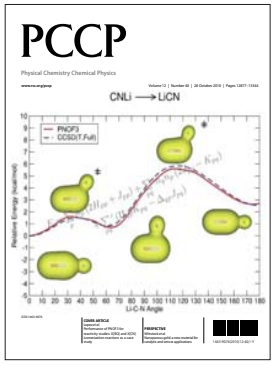
a) Optical extinction spectra of a nanoshell dimer bridged by a conductive molecular junction of radius a = 2nm as conductivity is increased via the increment of conductance. We can observe the variations in the behaviour of the plasmon resonance (BDP) and the emergence of the new resonance (CTP) in the IR part of the spectrum. b) Near-fields patterns corresponding to the short wavelength regime (top and middle) and to the long wavelength regime (bottom), where the progressive expelling of the electric field out of the junction can be observed.

High-frequency optical transport addressed optically.

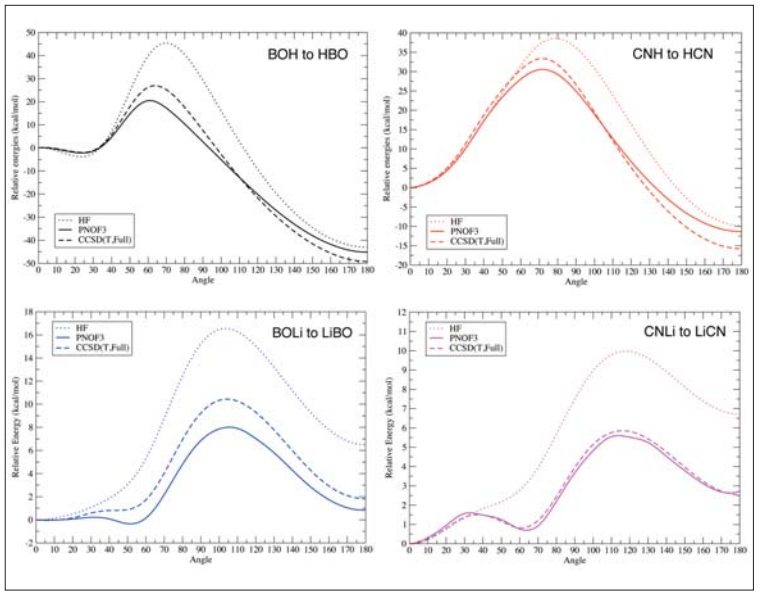
Performance of PNOF3 for reactivity studies: X[BO] and X[CN] isomerization reactions (X H, Li) as a case study

X. Lopez, M. Piris, J.M. Matxain and J.M. Ugalde
Physical Chemistry Chemical Physics 12, 12931-12934 (2010)

Natural Orbital Functional Theory in its PNOF3 implementation is used to investigate the potential energy surfaces of four isomerization reactions: (i) BOH to HBO; (ii) BOLi to LiBO; (iii) CNH to HCN; and (iv) CNLi to LiCN. These reactions are taken as a case study to illustrate the potentiality of PNOF3 to yield the correct topology for reactions sensible to electron correlation. The perfomance of PNOF3 to yield accurate reaction barriers and isomerization energies is also discussed. We have found that PNOF3 shows promising behaviour in the description of these delicate PESs, and yield the correct trends in isomerization energies and reaction barriers, although the latter trends tend to be somewhat lower than the ones calculated at highly correlated levels of theory. The present results show that PNOF3 can give a balanced description of electron correlation in both equilibrium and non-equilibrium structures.



Natural Orbital Functional Theory in its PNOF3 implementation is able to describe reactions with outstanding chemical accuracy in equilibrium and non-equilibrium structures that are highly sensible to electron correlation.



Potential Energy Surfaces as a function of the XBO and XCN (X=H,Li) angle. Results obtained from single-point PNOF3 and CCSD(T,Full) energies at the CCSD partially optimized geometries with XBO/XCN angle frozen at values that range from 0° to 180° with 10° variation. All calculations were done with the cc-pVTZ basis set. The relative energies, in kcal/mol, are calculated with respect to the energy of the 0° structure. Notice the good perfomance of PNOF3 in describing the topology of the four PES's.

Mixed-valency signature in vibrational inelastic electron tunneling spectroscopy

M. Alducin, D. Sánchez-Portal, A. Arnau, and N. Lorente
Physical Review Letters 104, 165423 (2010)

The unexplained vibrational inelastic electron tunneling spectroscopy (IETS) of O_2 on Ag(110) is now solved. When semilocal density functional theory is corrected by including static intra-atomic correlations, the IETS simulations are in excellent agreement with the experiment. The projected density of states revels that when adsorbed along the [001] direction, O_2 on Ag(110) is a mixed-valent system, where a spin-polarized molecular orbital dominates the electronic structure at the Fermi.

Inelastic electron tunneling spectroscopy (IETS) performed with the scanning tunneling microscope (STM) has given us unprecedented insight into the chemical structure of matter on the atomic scale. In the STM, electrons are tunneled through the vacuum gap between the tip and the substrate by applying them a bias voltage. Locating the tip over a single acetylene molecule adsorbed on a copper surface, Stipe, Rezaei and Ho showed that the tunneling electrons can give energy to the molecule and excite a particular vibrational mode. Since then, many experiments have confirmed the STM-IETS as a unique technique in which the vibrational spectra of individual adsorbates can be recorded by varying the tip-substrate voltage and used it as a fingerprint to identify the adsorbed species.

In general, the IETS signal corresponds to an increase of the STM conductance just at the energy threshold of the vibration because the excitation of a vibrational mode opens an additional channel for conduction. Interestingly enough, experiments performed for oxygen molecules adsorbed on a silver substrate showed that this picture, i.e., the conductance increase, does not apply in this case. Specifically, when the molecules are chemisorbed along the [001] direction on Ag(110) instead of increasing, the current decreases at the vibrational threshold of the stretching mode. These experiments had remained unexplained during years, since all the most sophisticated IETS simulations done on this system had been unable to reproduce the conductance decreases.

The IETS simulations performed by researchers at the DIPC that were published in Physical Review Letters have solved this long-standing puzzle. When semilocal density functional theory is corrected by including static intra-atomic correlations (DFT+U), the IETS simulations are in excellent agreement with the experiment. The analysis of the projected density of states shows that intra-atomic correlation leads to the spin splitting of the π_g orbital and the subsequent pinning of one of these orbitals to the Fermi level. The unforeseen consequence of our calculations is that when adsorbed along the [001] direction, O_2 on Ag(110) is a mixed-valent system in which a localized spin polarized orbital is at resonance with the Fermi level. The corresponding electronic structure leads to IETS simulations where the experimental change in conductance and also their spatial tip-position dependence are finally explained. The theoretical results give unprecedented information on the electronic and vibrational symmetries at work in this system. Importantly, these calculations also show that IETS can reveal important information about the electronic structure and magnetic nature of chemisorbed molecules. In this respect, IETS arises as a promising tool to characterize the otherwise elusive molecular mixed-valency regime. In this regime, electron correlations are responsible of large charge fluctuations between the adsorbate and the substrate that may lead to strong non-adiabatic effects dominating the adsorption dynamics.

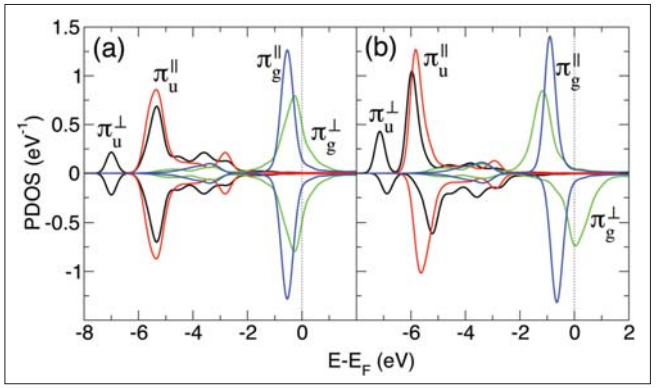


Figure 1. Spin-up (positive) and spin-down (negative) projected density of states of O_2 chemisorbed along the [001] direction. (a) Semilocal DFT (GGA) results. (b) Semilocal DFT+U (GGA+U) results.

STM operating in IETS mode arises as a promising tool to characterize the otherwise elusive molecular mixed-valency regime.

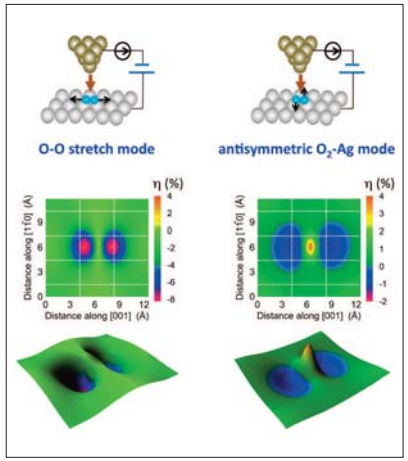


Figure 2. Semilocal DFT+U simulations of the spatial distributions of the conductance changes for the O-O stretch mode (left)and the antisymmetric O_2/Ag mode (right).

The unforeseen consequence of these calculations is that when adsorbed along the [001] direction, O_2 on Ag(110) is a mixed-valent system.

Theory of microwave-assisted supercurrent in quantum point contacts

F.S. Bergeret, P. Virtanen, T.T. Heikkilä, and J.C. Cuevas
Physical Review Letters 105, 117001 (2010)

In this work we presented a microscopic theory of the effect of a microwave field on the Josephson current through a quantum point contact. Our findings are important for the description of experiments that aim the manipulation of the quantum state of such structures.

The DC Josephson effect is one of the most striking examples of macroscopic quantum coherence. In the context of superconductivity this phenomenon manifests as the flow of a dissipationless DC current through a junction in the absence of any voltage. Since its discovery in the early 1960s, this effect has been observed in a large variety of weak links such as tunnel junctions, microbridges, atomic contacts, carbon nanotubes, semiconductor nanowires and graphene. If the constriction is shorter than the mean free path, the Josephson current is carried exclusively by a single pair of Andreev bound states (ABSs). There are some proposals of using the ABSs of a quantum point contact as the two states of a quantum bit. Since the two ABSs carry opposite supercurrents, the quantum state of the quantum bit can be probed, in principle, by means of current measurements. This led us to the central questions of our work: Is it possible to probe the ABSs by means of microwave spectroscopy? , and, how does a microwave radiation modify the supercurrent of a single-channel quantum point contact? Our theory based on the Keldysh technique demonstrates that indeed a microwave field can be used in order to probe the ABSs and predicts the following novel effects: (i) at low temperatures, the dc Josephson current can be strongly suppressed at certain values of the phase due to resonant microwave- induced transitions between the two ABSs (processes of type a and b in Figure 1). (ii) As the radiation power increases, the supercurrent-phase relation is strongly modified and it can even reverse its sign. (iii) At finite temperatures, the radiation can induce the transition of quasiparticles from the continuum to the lower ABS leading to an enhancement of the critical current as compared to the case in the absence of microwaves (process of type c in Fig 1). Our results are of relevance for many different types of weak links and in particular, they can be quantitatively tested in the context of atomic contacts.

Control and manipulation of the quantum state of a two-level system.

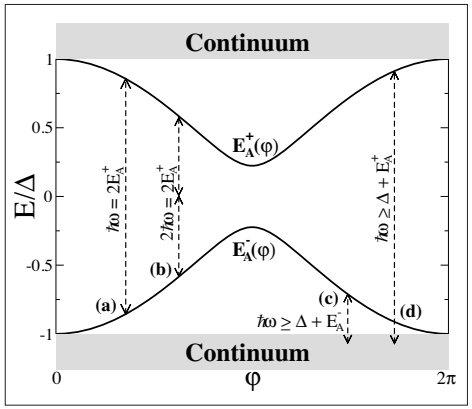


Figure 1. Dispersion relation of the Andreev Bound States in a single-channel QPC. The vertical dashed lines indicate one- and two-photon transitions between the ABSs (a-b), and transitions between the continuum and ABSs (c-d). The Fermi energy is at E=0.

Probing the Andreev Bound States through microwave spectroscopy.

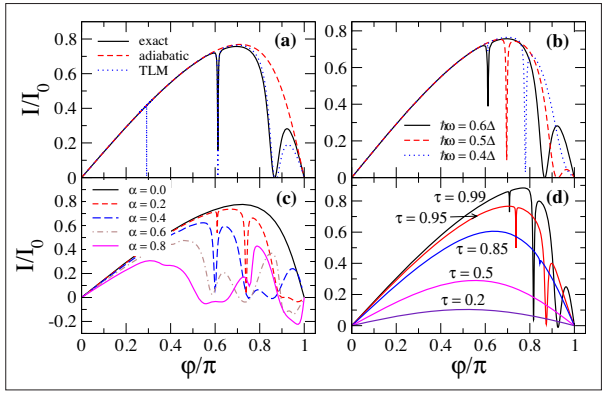


Figure 2. Zero-temperature dc Josephson current in the presence of a microwave field as a function of the phase difference through a quantum point contact with transmission 0.95. (a) The solid line shows the exact result while the dashed line corresponds to the adiabatic approximation. The dotted curve has been obtained from an effective two-level model. Rest of the panels show the exact result for (b) and different frequencies, (c) different microwave power and (d) different transmission of the contact.

Rare-earth thin film alloying: a new phase for $GdAu_2$

M. Corso, M. J. Verstraete, F. Schiller, M. Ormaza, L. Fernández, T. Greber, M. Torrent, A. Rubio, and J. E. Ortega
Physical Review Letters 105, 016101 (2011)

In this work we address the geometric and electronic structure of a new family of surface compounds formed by reactive deposition of rare-earth (RE) materials onto noble metal (NM) surfaces, forming a RE-NM_2 alloy. For the example of $GdAu_2$ we combine experimental end theoretical investigations to disentangle its atomic and electronic properties. In particular, the stacking of the bilayer allows for gadolinium's natural ferromagnetic state, at variance with the bulk phase, where frustration leads to antiferromagnetic interlayer coupling.

Many of the greenest technologies of the age, from electric cars to efficient light bulbs to very large wind turbines and future magnetic refrigeration, are made possible by an unusual group of elements: the rare earths (REs). The rare earths possess exotic electronic structure and delicately changing bonding, due to the presence of shallow and interacting *d*- and *f*-electron levels. These electrons are responsible for high and specific catalytic activities, remarkable alloying in metals, and specific luminescent properties. Precisely this richness, and the associated complexity, makes the determination of the structure and properties of RE materials very challenging. The REs demonstrate varying magnetism, coordination, oxidation states, and bonding types, as a function of the number and localization of the *f*-band electrons.

Prototypical and extremely rich RE systems are created by the alloying of gadolinium with *d*-band metals, and, in particular, gold and silver. These systems present magnetism, Kondo phenomena, and crystal structures that are tunable, depending on the precise alloy and on the RE content. Gadolinium is a borderline rare earth, which is naturally ferromagnetic but can easily switch to different magnetic states depending on the coordination (surface and cluster structure). Surface alloying introduces further degrees of freedom, and can give rise to novel phases. Here we study a new surface compound created by reactive epitaxy of Gd on a Au(111) crystal. Angle-resolved and core-level photoemission (ARPES, XPS) and scanning tunnelling microscopy (STM) demonstrate that a layer-by- layer growth of a stoichiometric $GdAu_2$ alloy occurs under particular conditions of Gd vapor flux and substrate temperature. Our theoretical analysis determines a particular layer stacking and magnetic ordering, at variance with bulk $GdAu_2$ crystals. Moreover, the experiment and theory feedback allows the characterization of the nature of electron bands, and, in particular, explains the exotic tip-height-dependent image contrast observed in STM.

Figure 1 shows how angle-resolved photoemission reveals the change in the electronic structure from Au to 1 and 2 monolayer thick $GdAu_2$ compound layers. One can observe new electronic Gd-derived electronic bands and the disappearance of the gold ones. Together with first principle DFT calculations and X-ray photoelectron diffraction investigations, the last ones carried out in collaboration with the University of Zurich, Switzerland, we determine the $GdAu_2$ layer stacking, which differs from that of bulk alloys. As proved by the theory, such distinct packing explains the surprising tunnelling-current- dependent contrast observed in STM, which is shown in Figure 2. By fixing bias and varying the tip-surface distance (current) the different atomic species of the surface compound are separately revealed. Usually, contrast variation in STM is obtained as a function of the tip-surface bias, reflecting tunnelling into distinct atomic orbitals, whereas in the present case the contrast arises as a function of the tip-surface distance.

With this work we have shed new light on the complex electronic structure and geometry of RE-NM surface compounds and as a side-product create a new tool to investigate and understand different atomic species on surfaces.

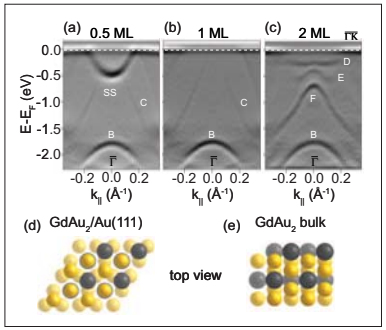


Figure 1. (a–c) Second derivative dispersion plots of the photoemission intensities corresponding to different Gd-Au sample preparations: (a) 0.5 ML $GdAu_2$/Au(111), (b) 1 ML $GdAu_2$/Au(111), and (c) 2 ML $GdAu_2$/Au(111). (d) Top view of the $GdAu_2$ bilayer, as determined in density functional theory. (e) Same for two (110) layers of bulk tetragonal $GdAu_2$.

We shed new light on the complex electronic structure and geometry of rare-earth–noble metal surface compounds, while predicting exotic magnetic properties.

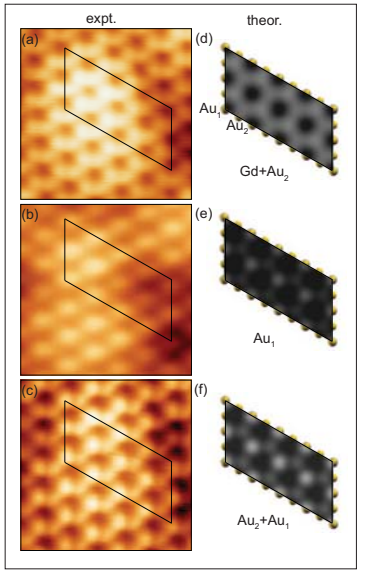


Figure 2. (a–c) High resolution STM images of the bilayer $GdAu_2$ surface compound, grown on Au(111). Three different atomic contrasts are measured by fixing the sample bias voltage (V_S) and tuning the tunneling current (I_T): (a) I_T=0.3 nA, (b) I_T=1 nA, and (c) I_T=2 nA. (d, e) Theoretical calculations allowing us to identify the different atomic species visible in (a–c) as indicated. Simulations are done at V_S=-1.2 V and decreasing STM tip-sample distance (dTS) from d_{TS}=5.19 Å in (d), to 2.61 Å in (e), and to 2.23 Å in (f).

Surveying molecular vibrations during the formation of metal-molecule nanocontacts

L. Vitali, R. Ohmann, K. Kern, A. Garcia-Lekue, T. Frederiksen, D. Sanchez-Portal, and A. Arnau
Nano Letters 10, 657-660 (2010)

Combined inelastic tunneling spectroscopy and first-principles calculations allow a precise characterization of the metal-molecule interaction during the formation of a metal-molecule nanocontact.

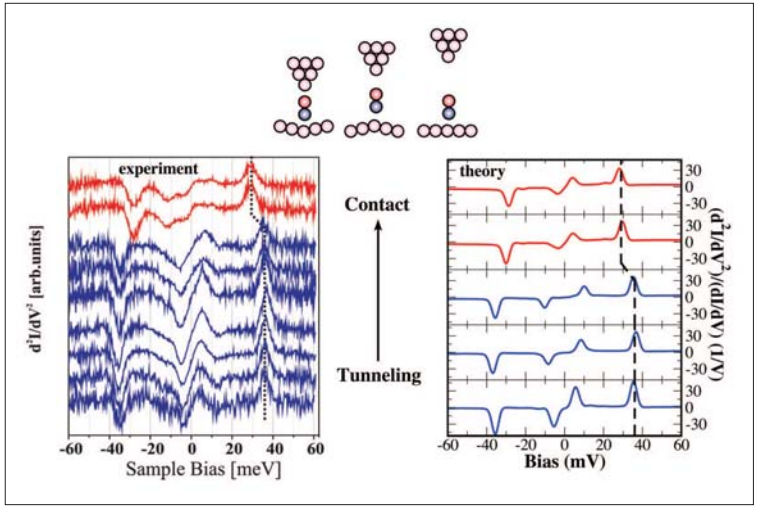
Charge transport through metal-molecule systems is a major subject of study in a rapidly growing interdisciplinary research field. It deals with fundamental and applied aspects of science at the nanoscale aiming to control the electron conductance at the molecular level and the uprising of nanotechnology. Within this context, accessing the influence of the molecular contact to the metal in the transport properties as metal-molecule systems are tuned from tunneling to contact is vital.

Experimentally, the metal-molecule coupling can be characterized through the spectroscopic signals of the molecular vibrations as measured by inelastic electron tunneling spectroscopy (IETS). This can be recorded as a function of the tip-molecule distance allowing understanding to which extent the contact formation influences the molecular properties. Further comparison with first-principles based simulations allows to achieve a deep understanding of the variation of the metal-molecule coupling as the tip-molecule distance decreases.

A good molecular prototype to study the influence of the metal-molecule bond is carbon monoxide (CO). For this reason, we have used the IETS signal measured at various molecule-metal distances by approaching the tip of an STM to the CO molecule adsorbed on a Cu(111) metal surface. The vibration modes of CO have been surveyed with unprecedented accuracy, and the following main observation has been made: a continuous but nonlinear blue shift of the frustrated rotation mode in tunneling with decreasing distance followed by an abrupt softening upon contact formation.

To obtain physical understanding of the experimentally observed frequency shifts, we have modeled the vibration modes and the inelastic transport using density functional theory (DFT) combined with nonequilibrium Green's function methods. Our calculations yield shifts for all these vibration modes along the transition from tunnel to contact, i.e., a clear indication of the existence of an appreciable tip-sample interaction.We assign the observed shifts to a modification of the surface potential under the influence of the tip proximity, as the tip-molecule distance is reduced. The interaction between them passes progressively from the attractive to the repulsive regime. Our results further indicate that the presence of the metal electrode sensibly alters the structural and conductive properties of the junction even without the formation of a strong chemical bond.

In conclusion, changes in the molecular vibrations give evidence of a perturbation of the electronic and structural properties of the junction as the STM tip approaches a single molecule. The observation of their shift is therefore a powerful tool to monitor the formation of a metallic nanocontact. We believe that these results have a general validity to the measurements of conductance through molecular junctions and might therefore clarify a few of the uncertainties in the electron transport through nanometer scale junctions.



Left panel: Measured vibration spectra for individual CO molecules on a Cu(111) surface at different tip-sample distances ranging from tunneling to point contact. The dotted black lines highlight the shift of the frustrated rotation (FR) mode vs the tip position. Right panel: Calculated spectra taken on top of a CO molecule adsorbed on a Cu(111) surface at different tipsample distances. A clear shift (red dotted lines) to lower energies is seen in the FR mode where the peak positions shifts from 35 to 29 meV as point contact is approached from tunneling, in close agreement with experiments. Upper panel: sketch showing the geometry of the junction and the relaxation of the sample under the influence of the tip proximity.

Shifts of the molecular vibration modes: fingerprints of metal bond formation.

Many-body effects in the excitation spectrum of a defect in SiC

M. Bockstedte, A. Marini, O. Pankratov, and A. Rubio
Physical Review Letters 105, 026401 (2010)

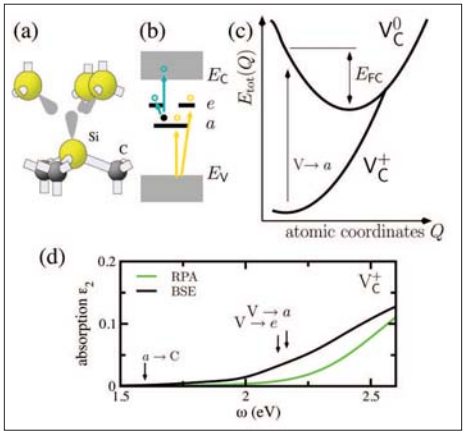
Researchers from the Donostia International Physics Center, the Center of Materials Physics (CISC) and the universities of Rome (Italy) and Erlangen-Nuremberg (Germany) demonstrated that the photophysics of the carbon vacancy in Silicon Carbide with two excitation channels involving conduction and valence bands is controlled by many-body effects beyond standard density functional theory through both the renormalization of the quasiparticle states and excitonic effects. Their analysis reassigns the excitation mechanism at the excitation thresholds observed in photoinduced paramagnetic resonance experiments.

Optical spectra of solids are comprised of the excitations of the perfect crystal and of its omnipresent imperfections. For instance in transparent metal oxides small abundances of point defects absorb light in the visible range and thereby determine the color of the material. Defects recently came into focus as a promising implementation of quantum bits for the realization of solid state quantum computers. The quantum information stored in the defect spin state is read out via an optical excitation.

Point defects as sources and sinks of charged carriers are fundamental for semiconductor technology without which modern world would not take place. In the investigation of novel materials for electronics, experiments unravel the role of specific defects via electronic and optical defect signatures. Unambiguous interpretation of the experiments and the assignment of microscopic defect models, however, requires theoretical support. Quantitative defect theory with density functional theory as its work horse successfully addressed the ground state defect physics and defect kinetics. Without being able to treat the excited state this work horse also notoriously underestimates semiconductor band gaps, thus, also affecting the prediction of defect level positions. Many-body perturbation theory is free from this error. The quantitative prediction of absorption spectra of a wide class of systems from insulators to surfaces, to nanotubes and polymers in this frame work became tractable only recently.

The international research team of the Donostia International Physics Center and the Center for Materials Physics (CSIC), and Universities of Rome (Italy) and Erlangen-Nuremberg (Germany) addressed this problem for a prototypical defect within the frame work of many-body perturbation theory by solving the Bethe-Salpeter equation and accounting for the GW self-energy. They selected the carbon vacancy in silicon carbide for its well-established identification and the extensive experimental investigation of the excitation spectrum of the positively charged defect. For the accurate interpretation of the experiments at least two competing excitation channels are relevant: electron transitions from valence bands to localized defect levels as well as transitions of defect electrons to conduction bands. Defect excitations combine the many-body effects in both extended and localized states. Electron insertion into defect states invokes on-site correlation due to electron-electron repulsion (Hubbard U), and defect-to-band transitions involve an electron and a hole (one in the localized state and the other in the extended state), thus adding excitonic effects.

In their full fledge GW+BSE calculations of the photophysics of the carbon vacancy the authors demonstrated that experimental spectra cannot be interpreted correctly without the inclusion of many-body effects beyond the density functional theory. Excitation spectra are red shifted by strong excitonic effects (~0.23eV) and electron-electron repulsion is underestimated by 0.3eV. Among the two competing excitation channels only the transition of defect electrons to the conduction band has photon energies in the range compatible with the absorption thresholds observed in the experiments. The theoretical analysis unambiguously rectifies the earlier experimental assignment of the excitation mechanism and assessment of ionization levels. These are pivotal for the defect diffusion and for understanding the carrier compensation in high purity semi-insulating SiC.



Excitation channels of the positively charged carbon vacancy in SiC: (a) geometry with sketch of spin density of the paramagnetic electron. (b) defect levels within the band gap. In the ground state the *a* level is occupied with one electron. Arrows indicate transitions form valence bands (V→*a*/*e*, lower set) and to conduction bands (*a*→C, upper set). (c) sketch of the total energy of the positive (V_C^+) and neutral (V_C^0) vacancies vs. the atomic coordinates. The transition V→*a* transforms V_C^+ into V_C^0 with a bound hole in the valence band. The occupation of the defect level implies additional relaxation (Franck-Condon shift). (d) Absorption spectra with and without excitonic effects at the BSE and RPA level extrapolated to high k-point densities and including the effect of Franck-Condon shifts. The transitions to the conduction bands sets in at lower photon energies than the transitions from the valence bands.

Excitonic red shifts and efect electron correlation are indispensible for unraveling the effect of competing defect excitation channels.

Magnetism of substitutional Co impurities in graphene

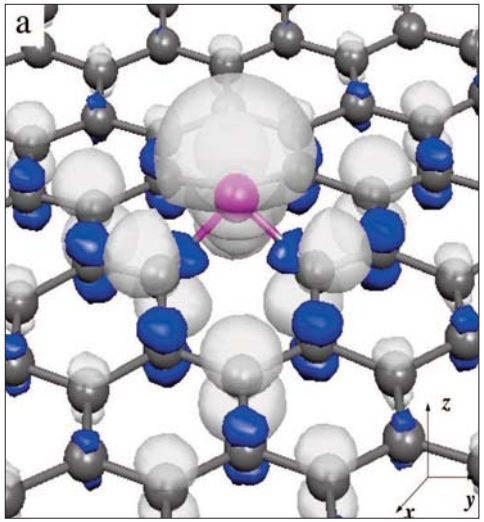
E.J.G. Santos, D. Sánchez-Portal, and A. Ayuela
Physical Review B 81, 125433 (2010)

We report *ab initio* calculations of the structural, electronic, and magnetic properties of a graphene monolayer substitutionally doped with Co (Co_{sub}) atoms. Our results show the complex magnetism of Co substitutional impurities in graphene, which is mapped into simple models such as the π-vacancy and Heisenberg model. The links established in our work can be used to bring into contact the engineering of nanostructures with the results of models in defective graphene.

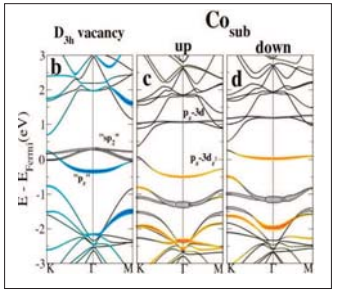
The peculiar electronic and magnetic properties of graphene monolayers have recently attracted much attention. New types of electronic and, particularly, spintronic devices based on graphene have been proposed. These graphene structures also drive an increasing interest to study defects, which are always expected in real-life devices. Intrinsic defects have been already widely studied and extrinsic defects, such as substitutional atoms, are presently under intense research. In spite of the growing interest about substitutional defects in graphene, little is known on magnetic properties such as spin polarizations and couplings.

In this work, we present a study of the structural, electronic, and magnetic properties of substitutional Co atoms in a graphene monolayer. We show that Co has spin polarization. This is in contrast to Ni substitutions which surprisingly do not show spin polarization. We observe that there is a one-to-one correspondence between the expected behavior for single vacancies in a simple-tight-binding model of graphene and that found for the Co_{sub} defects. The Co atom stabilizes a symmetric structure of the carbon vacancy. The electronic structure of the Co_{sub} defect at the Fermi energy E_{Fermi} is dominated by a single level with a strong contribution from the p_z orbitals of the neighboring C atoms. Each Co_{sub} defect shows a spin moment of 1.0 m_B . The total spin, however, follows closely Lieb's theorem for bipartite lattices and depends on the number of Co substitutions in each sublattice. Thus, magnetic couplings are predominantly anti ferromagnetic for Co_{sub} defects sited in the opposite same sublattice. Our calculations also show the dependence of the couplings on the crystalline direction and relative position of the defects.

Co_{sub} impurities in graphene as a realization of single vacancies.



Isosurface of the spin density induced by a Co_{sub} defect. Positive and negative spin densities correspond to grey and blue surfaces with isovalues of 0.008 e^- /$Bohr^3$, respectively. Panel b presents the spin-unpolarized band structure of an unreconstructed D_{3h} carbon vacancy. Panel c and d show, respectively, the majority and minority spin band structure a Co_{sub} defect in a similar cell. The size of cyan symbols in panel b indicates the contribution of the p_z orbitals of the C atoms surrounding the vacancy, whereas empty circles correspond to the sp^2 character. In panels c and d , the size of filled and empty circles denote the contribution of hybridized Co $3d_{z2}$-C $2p_z$ and Co 3d-C $2sp^2$ characters, respectively. E_F is set to zero.



Direct observation of confined single chain dynamics by neutron scattering

J. Martín, M. Krutyeva, M. Monkenbusch, A. Arbe, J. Allgaier, A. Radulescu, P. Falus, J. Maiz, C. Mijangos, J. Colmenero, and D. Richter
Physical Review Letters 104, 197801 (2010)

Neutron spin echo on entangled polymer chains confined in cylindrical nanopores has revealed direct microscopic measurement of the entanglement distance under confinement. This work constitutes the first experimental microscopic evidence of the dilution of the total entanglement density in a polymer melt under strong confinement.

Confinement effects in polymer melts may lead to unusual properties. This concerns both the chain conformation, which may be distorted in particular if the chain dimensions are significantly larger than the confinement size, as well as chain dynamics, which may be altered due to surface interactions and changes of topology and chain self-density. The understanding of such behavior is not only a scientific challenge but also important for knowledge-based applications in nanotechnology such as nanocomposites, coatings, adhesives, etc. Chain dynamics is commonly described in terms of the Rouse and the reptation model. In the Rouse model, the chain motion is determined by a balance of viscous and entropic forces. In addition, long polymers heavily interpenetrate each other and mutually restrict their motions *at long times* in forming topological constraints ('entanglements'). In the reptation model this effect is modelled by a tube of diameter d along the coarse grained chain profile confining the chain motion. The important question that is addressed now is how these dynamics change under confinement. Using the space-time resolution of neutron spin echo spectroscopy (NSE), in this work we realized the first direct observation of the entanglement distances and the associated intermediate scale Rouse dynamics under confinement conditions.

Poly(ethylene oxide) (PEO) confined in cylindrical nanopores of anodic alumina oxide (AAO) was investigated in samples where the chain dimensions (average bulk end-to-end distance) were either much larger or smaller than the lateral pore sizes. Mixtures of deuterated and protonated chains matching the scattering length density of the porous matrix were infiltrated. By means of small angle neutron scattering (SANS) we first determined the optimal experimental conditions to perform the dynamic measurements by NSE (see Figure 1).

Figure 2 shows the NSE results obtained for both samples. At intermediate timescales (Rouse regime) the data show a clear slowing down compared to the bulk behavior. This effect can not be related to a general increase of the friction between monomers, since in a previous work by other quasielastic neutron scattering techniques [1] the local dynamics at short times was found to be largely unchanged. At long times, the curves tend to finite plateaus that reflect confinement effects on the dynamics of the polymer chains -the single chain fluctuations are laterally restricted giving rise to a Debye-Waller type form factor. As can be seen in Figure 2 (a), the tube diameter deduced for the shorter (less-confined) chains is not appreciably influenced with respect to that found in the bulk (52 Å). The situation is different for the more confined long chains [Figure 2 (b)], where a 15% expanded entanglement network is observed. Thus, under strong confinement conditions the topological constraints imposed by the neighboring chains become diluted.

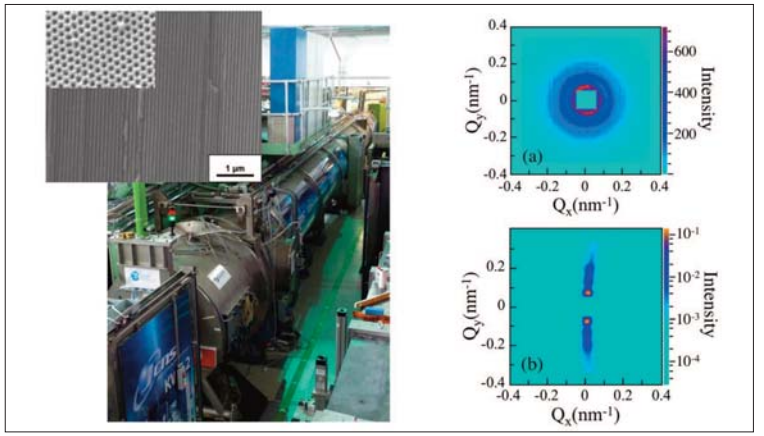


Figure 1. SANS results: (a) on the sample with the pores oriented parallel to the incident beam; (b) with the sample rotated by 15º around the vertical axis. Then, the cut of the inclined intensity sheet on the Ewald sphere becomes a circle and any residual scattering from the membrane occurs on the vertical axis. In the horizontal direction the scattered intensity is mainly due to the contrast between deuterated and protonated polymer chains revealing the chain structure factor. On the top, left: micrograph of the AAO templates.

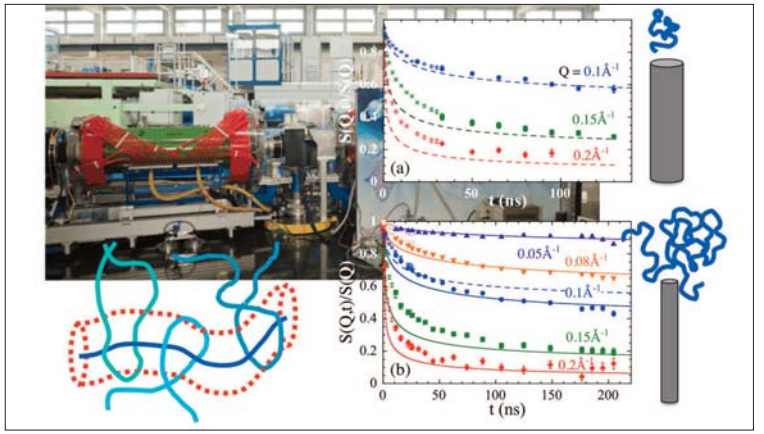


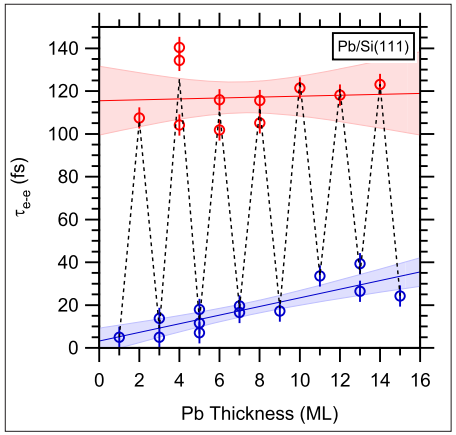
Figure 2. Normalized $S_{chain}(Q,t)$ of the short confined chains (a) and the long confined chains (b) at the Q-values indicated. Dashed lines: curves fitting the bulk PEO behavior with d = 52 Å [2]. Solid lines in (b): descriptions of the long-time plateaus, delivering a d^{conf}-value of 60.3 Å. The cartoon down on the left illustrates the tube concept (red dotted line) modeling the topological constraints imposed by the neighboring chains in the bulk.

Quasiparticle lifetimes in metallic quantum well nanostructures

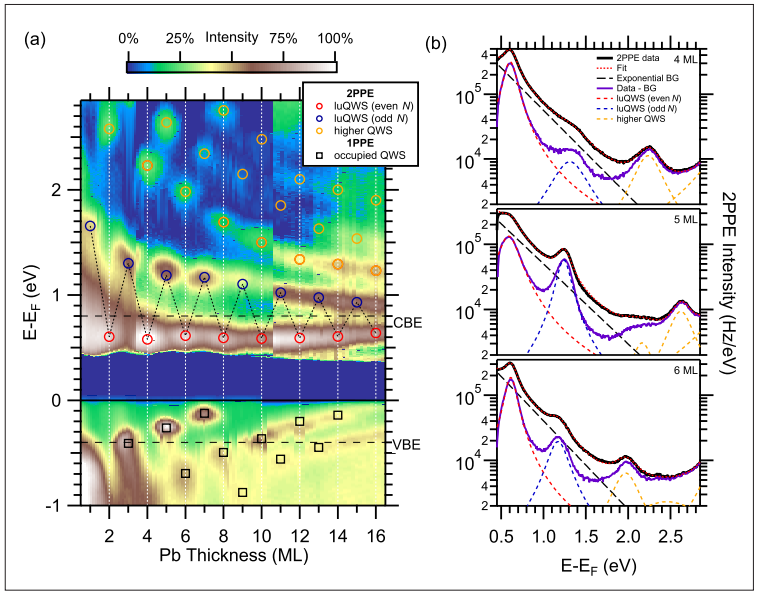
P.S. Kirchmann, L. Rettig, X. Zubizarreta, V.M. Silkin, E.V. Chulkov, and U. Bovensiepen
Nature Physics 6, 782 (2010)

Screening in bulk Pb is so much efficient that even ultrathin nanostructures of Pb obey the Fermi liquid theory.

Quasiparticle lifetimes in metals as described by Fermi-liquid theory are essential in surface chemistry and determine the mean free path of hot carriers. Relaxation of hot electrons is governed by inelastic electron–electron scattering, which occurs on femtosecond timescales owing to the large scattering phase space competing with screening effects. Such lifetimes are widely studied by time-resolved two-photon photoemission, which led to understanding of electronic decay at surfaces. In contrast, quasiparticle lifetimes of metal bulk and films are not well understood because electronic transport leads to experimental lifetimes shorter than expected theoretically. Here, we lift this discrepancy by investigating Pb quantum-well structures on Si(111), a two-dimensional model system. For electronic states confined to the film by the Si bandgap we find quantitative agreement with Fermi-liquid theory and ab initio calculations for bulk Pb, which we attribute to efficient screening. For states resonant with Si bands, extra decay channels open for electron transfer to Si, resulting in lifetimes shorter than expected for bulk. Thereby we demonstrate that for understanding electronic decay in nanostructures coupling to the environment is essential, and that even for electron confinement to a few ångströms the Fermi-liquid theory for bulk can remain valid.



Lifetime of the low unoccupied QWS as a function of Pb thickness. The solid lines are linear fits to guide the eye; the shaded areas indicate a 90% confidence interval of the fits. The error bars of the analysed electron lifetimes amount to ±5 fs and are determined by the statistical error of the data and the fitting procedure.



Quantized band structure of Pb/Si(111) for the occupied and unoccupied density of states at the Gamma point observed by photoemission. a) Photoemission intensity in a color map as a function of Pb thickness N in ML for the occupied and unoccupied quantum-well states (QWS) analysed by 1PPE and 2PPE, respectively. The 2PPE intensity is shown on a logarithmic scale, whereas the 1PPE intensity is plotted on a linear scale. The requirement that the sample work function is smaller than h**ν** in 2PPE prevented us from accessing energies E–EF <300 meV in these particular experiments. Red (blue) circles indicate the binding energies of the luQWS for even (odd) N; yellow circles indicate higher-lying QWSs. The binding energies are determined from a Lorentzian line fit as explained in b). The horizontal dashed lines indicate the positions of the valence- and conduction-band edges (VBE/CBE). The 2ML oscillation period of the binding energy of the luQWS is emphasized by a dotted line. The image is composed from three overlapping data sets; in total, 109 spectra have been analysed for this figure. b) 2PPE spectra for three exemplary values of N. The data are fitted by Lorentzian peaks and an exponentially decaying background (BG) and convoluted with a Gaussian instrument function. Background subtraction enhances the contrast between QWSs for odd and even N.

Atomic-scale engineering of electrodes for single-molecule contacts

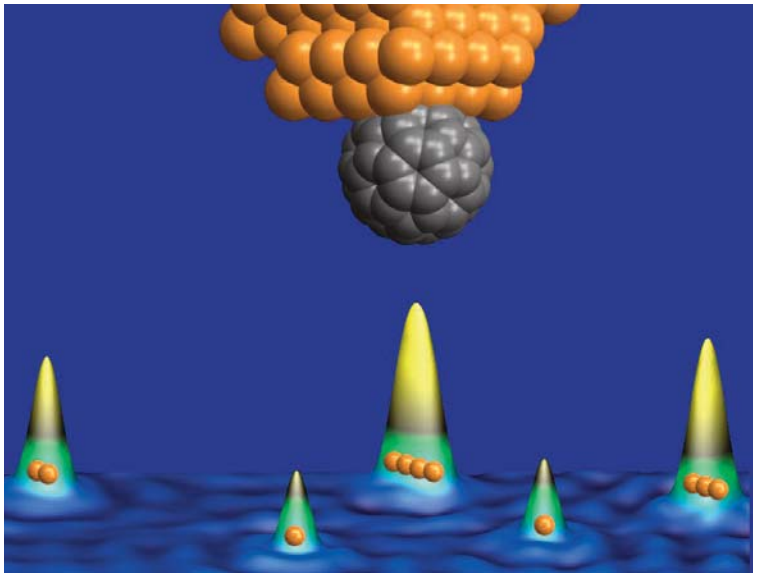
G. Schull, T. Frederiksen, A. Arnau, D. Sanchez-Portal, and R. Berndt
Nature Nanotechnology 6, 23–27 (2011)

Contacts between a single molecule and a metal electrode can be good or bad depending on the number of metal atoms that are in direct contact with the molecule.

One of the most challenging questions in novel molecular electronics is the fabrication of atomic-scale contacts to single molecules. This requires a precise and detailed characterization of the current flow in extremely small electrical circuits, so small that their components are individual atoms and molecules. It is precisely the small dimension of the system, typically in the nanometer range, that makes the solution difficult. In particular, for a junction formed by a single molecule the number of atoms making the contact, as well as their positions, are expected to be crucial parameters for its ability to conduct electrical currents. So far, there have not been any experiments where these variables have been controlled with sufficiently high precision.

Thanks to a collaboration between scientists in San Sebastian and Kiel (Germany) it is now been proven possible to determine and control the number of atoms making contact between a single C60 molecule and a copper metal electrode while the current flow through the junction is registered, as shown in the figure. In this way, these scientists have been able to quantify the changes in the electrical conductance across the molecular junction (metal/molecule/metal) as a function of the contact area between the molecule and the metallic electrodes. In brief, by changing the number of atoms in the contact one by one, it was found that there is a change from low (bad contact) to high (good contact) conductance. In the bad contact regime, the current flow is limited by the contact area, while in good contact regime the current flow is limited by scattering at the molecule.

Molecular contacts at hand.



Artistic representation of a scanning tunneling microscope (STM) tip with a C60 molecule at its apex suspended over a copper surface which has been manipulated at the atomic scale to accommodate clusters with different number of copper atoms. The copper clusters are used to make different contacts to the molecule by gently approaching the tip to each of them. The blue color surface in the lower part of the figure shows a real STM image of the metal surface with different number of copper atoms on top of it as indicated by the orange spheres [Image by G. Schull].

Plasmonic nanobilliards

P.E. Batson, A. Reyes-Coronado, R.G. Barrera, A. Rivacoba, P.M. Echenique, and J. Aizpurua
Nano Letters 11, 3388 (2011)

Optical forces have been studied for a long time in the context of trapping and manipulation of biological objects. Here the concept of plasmonic force is studied in the context of the interaction between a fast electron beam and metallic nanoparticles. Unexpected and novel forces are encountered.

Manipulation of nanoscale objects to build useful structures requires a detailed understanding and control of forces that guide nanoscale motion. We report here observation of electromagnetic forces in groups of metallic nanoparticles, derived from the plasmonic response to the passage of a swift electron beam. The nanophotonics research team at DIPC in collaboration with researchers at the university Autónoma of Mexico developed a theoretical framework that allows for calculation of the mechanical force induced at a metallic particle as a consequence of the polarization forces induced by a fast swift electron passing nearby. At moderate impact parameters of the electron beam, it is found that the forces are attractive, toward the electron beam, in agreement with simple image charge arguments. For smaller impact parameters, however, the forces are repulsive, driving the nanoparticle away from the passing electron. The repulsive force is an unexpected result originated by the excitation of high-order plasmons at the metallic particle that produce the repulsive effect. This control of the motion has been identified experimentally by researchers at the University of Rutgers, New Jersey, as shown in Figure 1. Both types of motion, attractive (A) and repulsive (B), have been monitored in a single gold nanoparticle thanks to the exquisite control of the electron beam impact parameter. The presence of a larger particle acts as a reference of the relative motion.

Furthermore, the presence of several metallic nanoparticles in proximity can provide a suitable platform to control and design plasmonic forces on demand. Particle pairs for example, are most often pulled together by coupled plasmon modes having bonding symmetry. However, placement of the electron beam between a particle pair pushes the two particles apart by exciting antibonding plasmonic modes. We suggest how the repulsive force could be used to create a nanometer-sized trap for moving and orienting molecular-sized objects, as shown in figure 2. The theoretical and experimental framework proposed in this work sets the basis for a kind of plasmonic nanobilliards, where the electron beam acts as the driving electrodynamical stick that hits the nanoparticles thanks to the Coulomb interaction in a very controlled manner, producing a broad set of dynamical events.

Swift electrons can produce novel forces that result in a controlled motion of metallic nanoparticles.

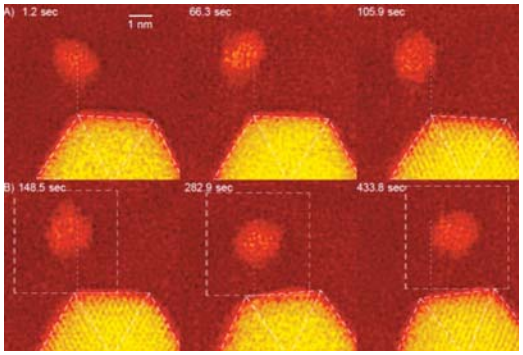


Figure 1. Experimental evidence of directed motion of a 1.5 nm Au particle on amorphous carbon. A) Pulling of a single sphere using a moderate, 4.5 nm, impact parameter. B) Pushing the same sphere using a 1 nm impact parameter. The scanning geometry was chosen to minimize forces between the 1.5 nm particle and the lager 4.5 nm particle that was used to allow measurement of the motion. Time stamps identify image frames. Experiments performed by Prof. P.E. Batson at IBM facilities and Rutgers University, New Jersey, USA.

Plasmonic forces can give rise to a rich dynamics of nanoobjects.

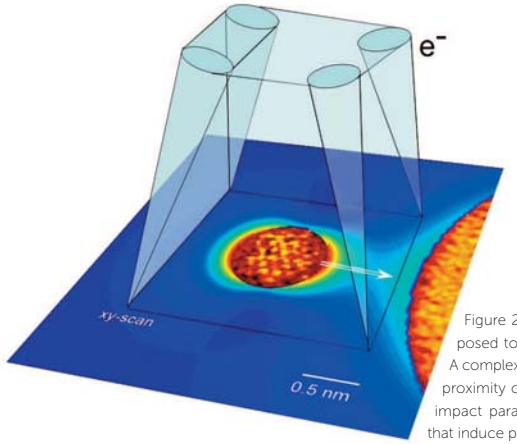


Figure 2. Schematics of the framework proposed to control the motion of nanoobjects. A complex beam of swift electrons travels in the proximity of metallic nanoparticles at a certain impact parameter producing plasmonic forces that induce particle motion.

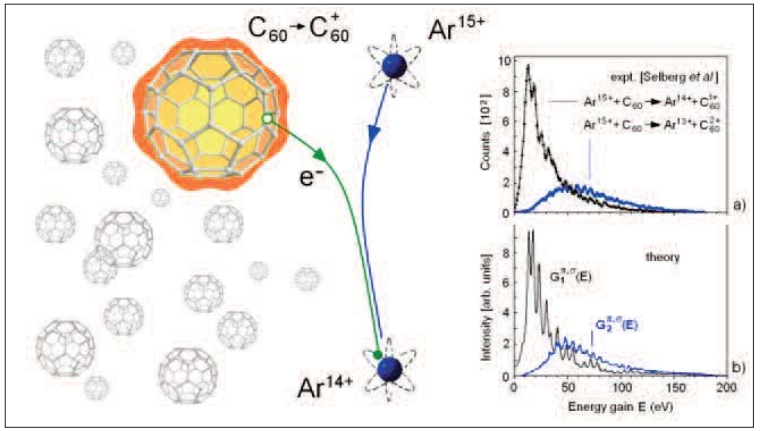
Quantum plasmon tsunami on a Fermi sea

Lucas, G. Benedek, M. Sunjic, and P.M. Echenique
New Journal of Physics 13, 013034 (2011)

A highly charged ion flying-by a fullerene molecule violently strips away one of its valence electrons leaving behind a plasmon quantum tsunami, consisting in a coherent state of excitations of the charge density. The electron transfer confers an energy gain to the ion minus the energy required to excite the plasmon coherent states. By explaining a 15-years-old conundrum raised by state-of-the-art scattering experiments, a team of researchers from DIPC and the Universities of Namur, Milano-Bicocca and Zagreb suggest a new tool to investigate energetic collective excitations in nanostructures.

A beam of energetic, highly charged Ar^{q+} ions is sent through a dilute C_{60} fullerene vapor. An ion, which happens to pass by a neutral molecule, strongly polarizes it to the point where it may capture one or several electrons which land onto the ion discrete Rydberg states (Figure). The electronic potential energy released by the charge transfer causes an increase of the ion kinetic energy: Some understanding of the basis of the mechanism was already pointed out some years ago however, the highly unexpected shape of the measured energy gain distributions could not find a straightforward explanation. The gain curves extend smoothly to very high energies and are topped, from beginning to end, by series of small oscillations of 6 eV period (see Figure inset (a)), which evidently bear very little relation to the underlying set of discrete ion Rydberg levels. The work summarized here demonstrates that the discrete Rydberg spectrum is the due to the occurrence of a plasmon tsunami on the molecule. This consists of a violent rearrangement of valence electrons around the positive hole left behind on C_{60} by the fast electron transfer. Charge density waves rush to screen the naked positive hole as it suddenly appears. This causes multiple plasmon excitations whose energy quanta are provided by the ion kinetic energy. The electrons always land on Rydberg levels but the energy liberated is apportioned between the ion kinetic energy increase and creations of plasmons. Thus the intensity of the kinetic energy gain peak, expected to appear at the nominal position of a Rydberg level, is in fact redistributed over a Poissonian series of plasmon peaks (hence the oscillations) extending on the loss side of the level.

The theory developed in this work convincingly accounts for the observed spectra for all momenta q, as shown in the Figure inset (b). The phenomenon is a real electrodynamical quantum tsunami on the molecule which rings like a bell whenever one or several of its electrons are stripped away by the ion. The experimental method of highly charged ion energy gain spectroscopy, supported by the new understanding of the present theory, offers a novel opportunity to investigate collective excitations in a variety of nanostructures such as large molecules, atomic clusters or solid surfaces.



A highly-charged argon ion, e.g., Ar^{15+}, when passing through C_{60} gas can fly by a molecule so as to violently strip away and capture one of its valence electrons (e^{-}). Charge density waves rush to screen the positive hole left behind on C_{60} thus raising a tsunami of coherent plasmon excitations (orange waves) whose energy quanta are provided by the ion kinetic energy. The ion gains the energy released by the electron in dropping into a Rydberg state of the ion, decrease however by the energy required to excite a coherent distribution of C_{60} plasmons. The gain spectra for one and two electron transfers measured by Selberg et al (inset (a)) are well reproduced by theory (inset (b)) once both π and σ plasmons of C_{60} are considered.

A highly charged ion strips away a valence electron from a molecule leaving behind a plasmon quantum tsunami.

Hierarchical selectivity in fullerenes: formation of C_{70}-amino acid chimeras

E.E. Maroto, A. de Cózar, S. Filippone, Á. Martin-Domenech, M. Suarez, F.P. Cossío, N. Martín
Angewandte Chemie 123, 6184–6188 (2011)
Angewandte Chemie International Edition 50, 6060–6064 (2011)

Selectivity is still a major challenge in fullerene research. In this paper, we describe how the use of suitable chemical and computational tools permit the preparation of C_{70}-proline chimeras with complete control, despite the inherent structural and electronic complexity of higher fullerenes.

Since the discovery of fullerenes and their further preparation in multigram scale, these molecular carbon allotropes have been thoroughly investigated from the chemical viewpoint in the search for new modified fullerenes able to exhibit unconventional properties for practical applications. Higher fullerenes include a great diversity of molecules with different structures and chemical behavior that, due to the minor degree of symmetry, give rise to a complex covalent chemistry where chirality is an important and fascinating aspect.

Unlike C_{60}, C_{70} lacks of a spherical symmetry and it has four different types of double bonds on the cage. Accordingly, additions occur preferentially at the most strained fullerene double bonds, namely those located at the polar zone (site α followed by β and γ sites, see Figure 1a). Within this context, we decided to explore the hierarchical selectivity of C_{70} in its transformation into unnatural proline derivatives. L-proline is the only natural amino acid whose five-membered cyclic structure involves the amino group, thus conferring this molecule with special structural features when it is forming polypeptides. These C_{70}-proline chimeric adducts should exhibit interesting properties.

We observed that the Fukui indexes predict the site-selectivity of C_{70} in these [3+2] cycloaddition reactions as well as the facial selectivity of the other reactant, a 1,3-dipole named azomethine ylide (Figure 1b). In addition DFT-based calculations predict correctly the regio- diastereo- and enantioselectivity of these stepwise reactions (Figure 2). It is interesting to note that our calculations also indicate that the metal-catalyst complex shows a lower affinity for the cycloadduct than for the starting azomethine ylide, thus allowing the completion of the catalytic cycle.

In summary, in this paper we have described for the first time the selective preparation of C_{70}-proline chimeric cycloadducts. In addition, the computational results and the model developed can be extended to other modified higher buckiballs whose preparations constitute a major challenge in fullerene research.

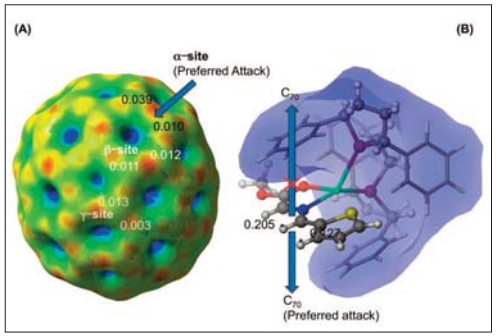


Figure 1. (A) Electrostatic potential projected on the electron density of C_{70} (B3LYP/LANL2DZ level of theory). Given numbers are the electrophilic Fukui indexes at the α–γ sites in arbitrary units. The higher the number, the higher the local electrophilicity. (B) Fully optimized silver azomethine ylide (B3LYP/LANL2DZ:PM6 level of theory) complexed with the catalyst. B3LYP and PM6 layers are represented in ball and stick and tube modes, respectively).

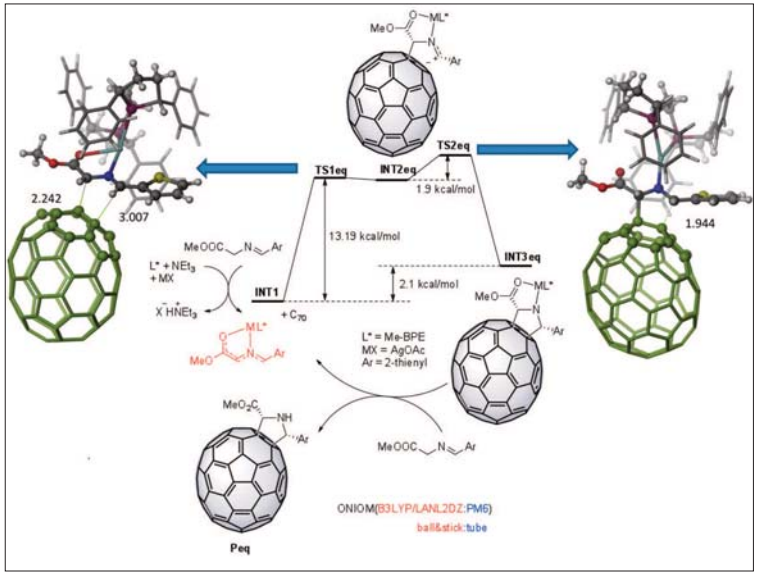


Figure 2. Reaction coordinate associated with the reaction between C_{70} and a model silver azomethine ylide. Relative energies were optimized at B3LYP/LANL2DZ//B3LYP/LANL2DZ:PM6 level of theory.

Anharmonic stabilization of the high-pressure simple cubic phase of calcium

I. Errea, B. Rousseau, and A. Bergara
Physical Review Letters 106, 165501 (2011)

The understanding of how the atoms vibrate in a solid is crucial to comprehend many of its physical properties. As an example we can cite thermal transport properties, specific heats, Raman and neutron diffraction spectra and the very appealing superconductivity. These atomic vibrations are generally explained in terms of phonons: the quantum of the atomic oscillations. Phonons are calculated in regular basis applying the harmonic approximation, that is, considering exclusively the behavior of the ionic potential in the vicinity of the equilibrium position. However, there are cases in which the behavior close to the equilibrium position does not describe properly the dynamical behavior of the solid and leads to wrong results. For example, there are experimentally confirmed structures of solids that display imaginary phonons in *ab initio* calculations suggesting that the crystal structure is unstable and cannot be realized experimentally. In order to solve this apparent contradiction the behavior of the atoms farther from equilibrium needs to be taken into account, that is, anharmonicity cannot be neglected in these systems.

The high-pressure simple cubic phase of calcium is a clear example of the latter. Although phonon calculations based on the harmonic approximation predict that this phase is unstable, many experiments confirm that this phase is stable and exists in nature. Moreover, calcium starts to superconduct in this simple cubic phase and becomes the element with the highest superconducting transition temperature (*Tc*) reaching 29 K above 200 GPa in another phase. Thus, the emergence of superconductivity in Ca cannot be understood within the harmonic approximation since the electron-phonon interaction cannot be calculated with imaginary phonons.

Considering that in the harmonic result the ground state energy is not bounded, the anharmonicity in simple cubic Ca requires a variational approach and suggests the application of the self-consistent harmonic approximation (SCHA). The SCHA assumes that the best phonons are those that minimize the free energy of the system. In order to apply the SCHA an arbitrary harmonic term is included and subtracted to the potential. Then, the free energy is minimized with respect to this arbitrary harmonic term. Finally, the frequencies that diagonalize the arbitrary harmonic part are the anharmonic frequencies. In order to do so, the anharmonic coefficients need to be known. In this work performed at the DIPC, this procedure has been applied for the first time using rigorous *ab initio* calculations.

The method that has been developed is able to predict that the simple cubic phase of calcium is stabilized by strong anharmonic effects. Moreover, the anharmonic phonon dispersion that has been obtained has made possible the calculation of the electron-phonon coupling and predict the superconducting properties of this system. The calculated value of *Tc* is in sharp agreement with recent experiments. This strongly supports the validity of the method used.

The SCHA is a theory that might be used to understand many systems were anharmonicity plays a crucial role such as ferroelectrics, systems with charge-density waves and hydrides. These results shows that the SCHA is an appropriate framework to tackle all these type of systems within *ab initio* calculations, something not possible so far.

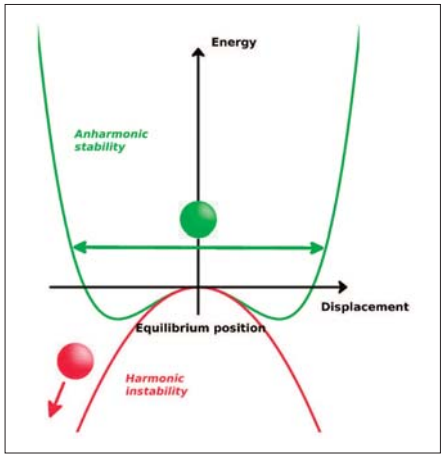


Figure 1: Schematic representation of how anharmonicity can stabilize the atomic vibrations and how the harmonic approximation can yield to a wrong interpretation.

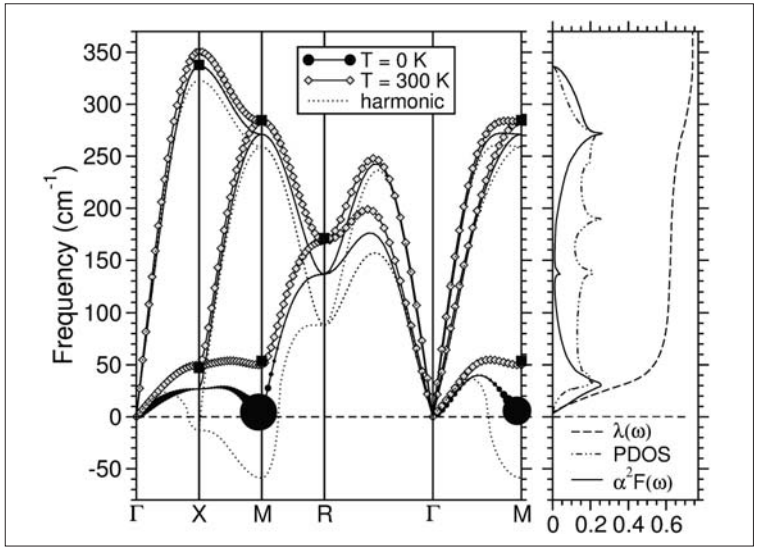


Figure 2: Harmonic phonon spectra and renormalized anharmonic phonon spectra at 0 and 300 K of simple cubic Ca at 50 GPa. The anharmonic results for the integrated electron-phonon coupling parameter, the Eliashberg function and the phonon density of states (PDOS) are shown as well.

Circular dichroism in laser-assisted short-pulse photoionization

A.K. Kazansky, A.V. Grigorieva, and N.M. Kabachnik
Physical Review Letters 107, 253002 (2011)

A remarkable effect of circular dichroism, i.e. a difference in photoelectron spectra produced by right and left circularly polarized light in two-color multiphoton ionization of atoms, is predicted for the case when the atom is ionized by an extreme ultraviolet or x-ray femtosecond pulse in the field of a strong infrared laser pulse, both pulses being circularly polarized.

Two-color multiphoton ionization experiments, in which an atom is ionized by an extreme ultraviolet (XUV) or x-ray photon in the presence of a synchronized strong field of femtosec- ond optical laser, have been successfully realized first with the XUV sources based on high harmonic generation. The laser-assisted XUV photoionization of atomic systems has been successfully used in time-resolved investigation of core-level relaxation dynamics. As an extension of these studies, two-color experiments at free electron lasers (FEL) have proved to be an effective method of studying photoionization dynamics as well as a useful instrument for characterizing the parameters of the FEL beams. In particular, the strong optical laser field modifies the photoionization continuum leading to formation of a sequence of sidebands in the photoelectron spectra which exhibit a strong dependence on the temporal separation, intensity and duration of the XUV and visible or infrared pulses.

One of the most effective methods of studying the photoionization is the investigation of the polarization effects and, in particular, of various types of dichroism (circular or linear) in photoelectron spectra. The dichroism is defined as the intensity difference in the electron emission for two different directions of either the polarization of the ionizing photons or of the target atom polarization. Studying dichroism in photoionization of polarized atoms with synchrotron radiation sources allowed one to obtain complete information on photoionization amplitudes including their phases. Circular dichroism in photoemission from solids has been widely used for investigation of local magnetization and other properties of solids and surfaces.

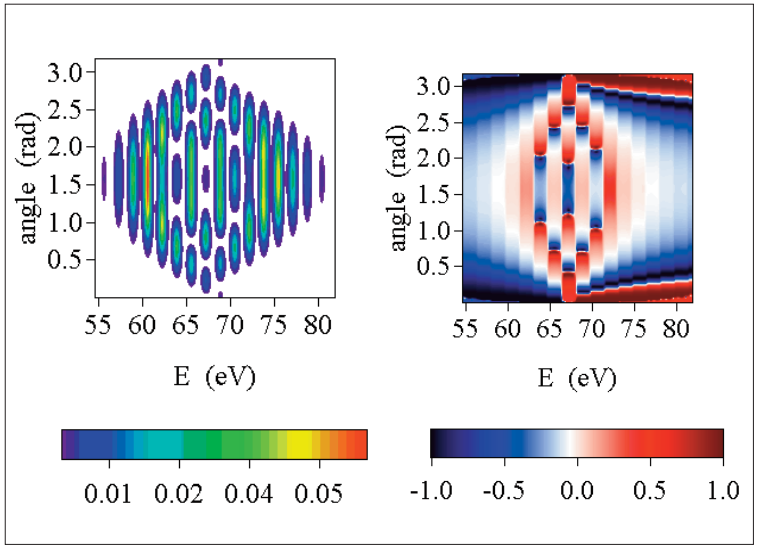
Up to now all FELs produce linearly polarized light. However, it is planned to obtain circularly polarized beams of XUV and x-ray radiation in the near future. Thus for planning future experiments it is timely to investigate theoretically the effects of circular polarization in two-color multiphoton ionization in conditions, which are characteristic for modern FELs.

In this Letter we predict a notable effect of circular dichroism (CD) in short-pulse photoionization by circularly polarized XUV or x-ray photons in the strong field of a circularly polarized optical laser. CD in photoelectron emission is defined as the difference in electron emission probability for right and left circularly polarized light.

We have calculated as an example the CD for ionization of He atom by the XUV pulse with energy of 92 eV and duration 2.4 fs in the field of IR laser (800 nm) with intensity of 3:5 1012 W/cm2 and pulse duration of 30 fs. At the chosen XUV photon energy the photoelectron energy (disregarding the effect of IR field) is 67.4 eV.

In Fig. 1 the two-dimensional color-scale plots present the calculated double-differential cross section (DDCS) (left panel) and the corresponding CD (right panel) as function of electron energy and emission angle. Red color shows positive CD (cross section for right circularly polarized XUV photons is larger than for left ones). Blue color shows negative CD. One can see that CD strongly varies from one sideband to another. The sidebands of the lowest order (close to the central line at 67.4 eV) exhibit large CD of alternating sign at any angle. In turn, each of the lower-order sidebands shows CD quickly varying with emission angle. Higher order sidebands exhibit small CD of negative sign, slowly varying with angle. We note that stripes of large CD at the angles close to zero and 180° have little meaning since the cross sections in these area are vanishingly small [see Fig. 1 (left panel)].

The predicted effect can be observed both in angle resolved and angle-integrated experiments. The CD effect can be used to measure circular polarization of the XUV or x-ray light in the energy region where other methods are not effective.



Left panel: DDCS calculated for photoionization of He by right-hand circularly polarized XUV photons at the energy 92 eV in the right-hand circularly polarized IR laser field (800 nm, 10^{12} W/cm^2). Other parameters see in text. Right panel: Dichroism calculated for the same parameters.

Quasiparticle interference around a magnetic impurity on a surface with strong spin-orbit coupling

A. Strózecka, A. Eiguren, and J.I. Pascual
Physical Review Letters 107, 186805 (2011)

On surfaces with strong spin-orbit coupling, back-scattering is forbidden since it requires flipping of the spin of the electron. It has been proposed that the forbidden scattering channels in such systems can be activated if time reversal symmetry is locally broken, for example, by a magnetic scattering center. Scanning tunneling spectroscopic maps of quasiparticle interference patterns around a single magnetic MnPc molecule on a Bi(110) surface reveal only spin-conserving scattering events. In this work we present a real space non-perturbative Green's functions approach, confirming that charge-density interference patterns are unaffected by the magnetic state of the impurity. A fingerprint of backscattering processes appears, however, in the magnetization patterns, suggesting that only spin-polarized measurements can access this information.

In this work we investigate electron scattering around a single magnetic molecule, a manganese phthalocyanine (MnPc), on a surface with strong SOC: Bi(110). Bismuth became recently a parent element for various topological insulators. Strong SOC in Bi surfaces causes large anisotropic spin splitting of its surface electronic bands and leads to a clear manifestation of spin-dependent scattering phenomena. Figure 1 shows the calculated band structure along high symmetry lines, the spin polarization of the surface states and the measured density of states.

We make use of a combination of FT-STM experiments with theoretical results considering fully relativistic non-collinear-spin spinor real space structure + 2x2 Spin Green's function approach (the first of this type). We demonstrate in particular that the magnetic moment of the scattering center has a negligible effect on the LDOS modulation around it. The corresponding QPI maps show no fingerprint of scattering violating TR symmetry revealing instead a clear dominance of spin-conserving scattering, similar to the case of nonmagnetic impurities. The simulations allow us to clearly identify the scattering processes suppressed by the spin polarization of the surface states and determine the interference patterns around a magnetic scattering potential.

An important results of this work is the prediction that a magnetic impurity with a well defined magnetic moment induces back-scattering in the system; the effects of it are, however, expected to be observed only in spin-resolved measurements. Figure 2 illustrates the calculated (the first of this type) reciprocal space magnetization pattern induced by a localized moment, demonstrating a clear enhancement of several areas of the Brillouin zone which are clearly suppressed for the case of the total charge modulation.

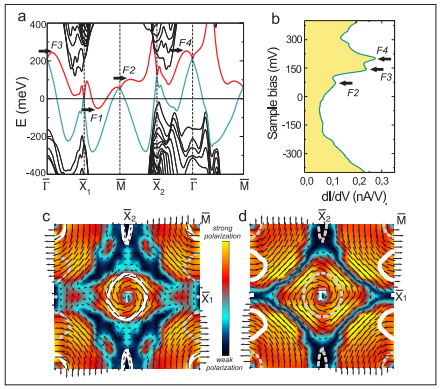
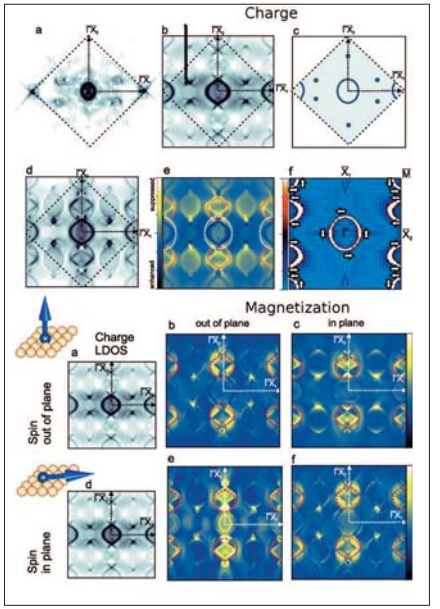


Figure 1. Electronic and spin structure of Bi(110) from first principles calculations. (a) Band structure of the surface electronic states. SOC splits the surface band into two sub-bands (red and blue). (b) dI=dV spectrum of a clean Bi(110) surface: Peaks F3 and F4 correspond to the spin-split top of the hole pocket at and peak F2 to the top of the pocket at M. (c), (d) Spin texture within the first surface Brillouin zone, for the lower and upper sub-band, respectively. The color code represents the degree of the spin polarization (see the text for details); arrows show the direction of the spin in the surface plane. The Fermi contour of the corresponding sub-band is superimposed on the plot as solid lines; the dotted lines depict the contribution from the other sub band.

Figure 2. FFT of charge and spin LDOS modulation around a magnetic scattering center for two different spin orientations: out of plane (a)–(c) and in plane (X2 direction) (d)–(f). The FFT of charge features similar to the case of nonmagnetic impurity. A clear fingerprint of scattering between states of opposite spin is identified in the magnetization patterns: (b),(e) out of plane and (c),(f) in plane.

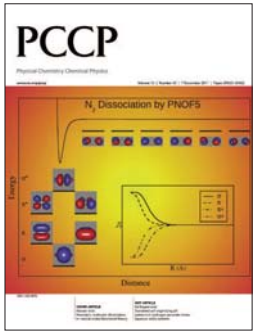


Spin conservation inducing a finite magnetization in a non-manetic material.

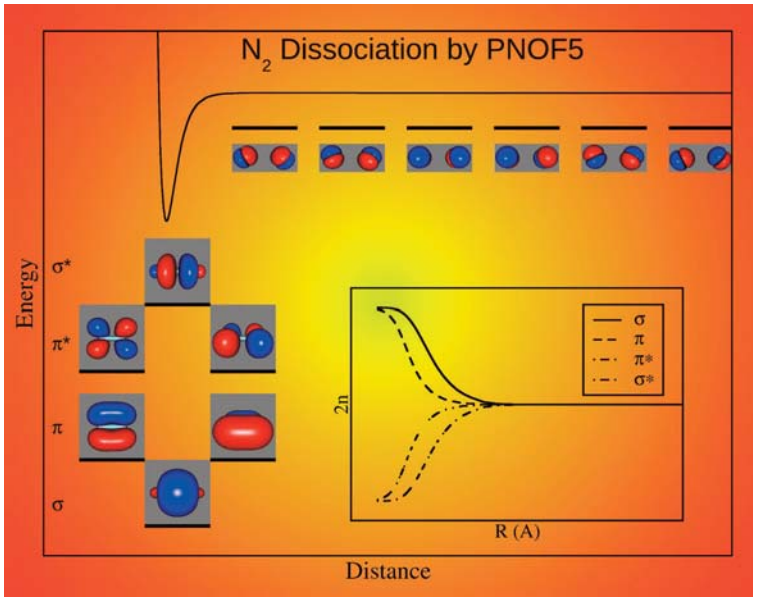
Homolytic molecular dissociation in natural orbital functional theory

J.M. Matxain, M. Piris, F. Ruiperez, X. Lopez and J.M. Ugalde
Physical Chemistry Chemical Physics 13, 20129 (2011)

The dissociation of diatomic molecules of the 14-electron isoelectronic series N_2, O_2^{+2}, CO, CN^- and NO^+ is examined using the Piris natural orbital functional. It is found that the method describes correctly the dissociation limit yielding an integer number of electrons on the dissociated atoms, in contrast to the fractional charges obtained when using the variational two-particle reduced density matrix method under the D, Q and G positivity necessary N-representability conditions. The chemistry of the considered systems is discussed in terms of their dipole moments, natural orbital occupations and bond orders as well as atomic Mulliken populations at the dissociation limit. The values obtained agree well with accurate multiconfigurational wave function based CASSCF results and the available experimental data.



Astonishing behavior of PNOF5 at the dissociation channel. It dissociates to integer number of electrons.



In this figure all the relevant information for the dissociation of N_2 is included. Note that the obtained Natural Orbitals are depicted at the equilibrium region and at the dissociation limit, and that the occupation numbers of such Natural Orbitals are depicted as a function of the interatomic distance. It is observed that at the dissociation limit all these orbitals have occupation number 1, and that Natural Orbitals are delocalized in both atoms, which corresponds to the correct dissociation to two atoms in their ground quartet states. Finally, the dissociacion curve is also provided.

PNOF5 accounts for non-dynamical electron correlation.

One dimensional bosons: from condensed matter systems to ultracold gases

M.A. Cazalilla, R. Citro, T. Giamarchi, E. Orignac, and M. Rigol
Reviews of Modern Physics 83, 1405-1466 (2011)

We review a century of both experimental and theoretical results on interacting bosons systems in one dimensions. We also discuss current problems and future challenges.

When matter is forced to move predominantly on a line, qualitatively new kinds of behavior emerge. At the individual level, we are all painfully familiar with this situation, as we experience it every time we are ourselves trapped in a traffic jam or we have to queue to buy movie tickets, for example. However, if we forget about the individual aspect of being forced to move on a line, we can easily grasp its collective side: in order to move (forward or backward), all individuals in the queue must agree to do so. This collectivizes any motion and turns it into a highly correlated phenomenon: if one individual moves, it is because all the others also do to some degree.

Indeed, microscopic particles like atoms or electrons, which behave according to the laws of Quantum Mechanics, also experience this kind of collectivization when they are confined to move on a line. Although this was theoretically discovered very early in the history of Quantum Physics, but for a long time the study of models of systems of quantum particles interacting on the line was regarded as a theorists' playground; It was a field for the more or less mathematically inclined theoretical physicists to occupy themselves trying to solve toy models, which -it was hoped- could shed light into the complexities of real materials where particles move in all three familiar dimensions of space.

Understanding the properties of matter confined in narrow channels is becoming more and more necessary as the size of elements of microchips is pushed towards the limits of miniaturization by the electronics industry. In the future, the properties of electronic devices, as well as the wires connecting them, will be strongly affected by quantum effects. This will lead to electronic "traffic jams", which make it difficult the transmission of currents in such devices, and which will also require the development of new devices that exploit the properties of one dimensional systems. Moreover, new materials with strong direction-properties may be created: For example, heat conductors that conduct heat very efficiently in only one direction while remaining cool (due to a poor heat conductivity) in the other directions.

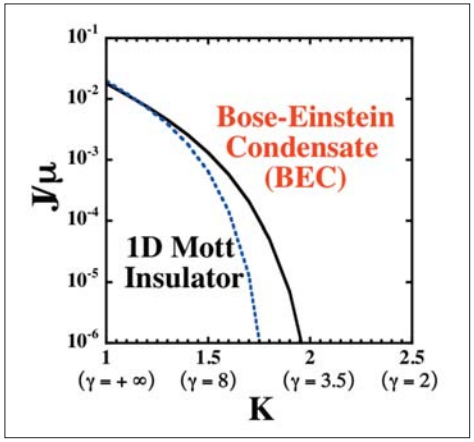


Figure 1. Phase diagram of a coupled 1D Boson system. K is a dimensionless parameter that Measures the strength of the interactions amongst the bosons in 1D. J is the strength of the Josephson coupling (quantum tunneling) between the the 1D systems.

Strongly anisotropic anomalous Hall effect in FePt ordered alloys

H. Zhang, F. Freimuth, S. Blugel, Y. Mokrousov, and I. Souza
Physical Review Letters 106, 117202 (2011)

Ferromagnets display a spontaneous Hall effect even in the absence of an applied magnetic field. We have studied this "anomalous" Hall effect in FePt ordered alloys by means of first-principles calculations, finding that its magnitude varies strongly with the orientation of the ferromagnetic moment relative to the crystal axes. The calculations reveal that the strong anisotropy is caused by the off-diagonal part of the spin-orbit interaction, which couples electron states with anti-parallel spins.

The Hall effect has played a central role throughout the development of condensed-matter physics. In its simplest form, it consists of a transverse voltage which develops in a current-carrying sample in crossed electric and magnetic fields. This "ordinary" Hall effect occurs in all metals as a result of the Lorentz force acting on the conduction electrons. In ferro- and ferrimagnetic metals, a Hall effect is observed even in the absence of a magnetic field. The origin of this anomalous Hall effect (AHE) is much more subtle, and has been a source of controversy for many decades. First-principles calculations carried out over the last ten years have helped clarify the microscopic origin of the AHE. It is now understood that the effect can be accounted for by a subtle modification to the velocity of the conduction electrons as they move through the periodic crystal in the presence of the relativistic spin-orbit interaction (SOI).

In previous theoretical studies it was commonly assumed that most of the AHE could be ascribed to the "spin-conserving" part of the SOI, which couples the components of the spin and orbital angular momenta along the magnetization direction. However, in reality the electron eigenstates in the crystal are not purely spin-up or spin-down: the nominally "up" states have in general a small "down" component, and vice-versa, as a result of the off-diagonal ("spin-flip") part of the SOI. The spin mixing can become particularly strong when two bands of opposite spin character cross and mix (Fig. 1). We have found that this mixed-spin character of the electron states leads to surprising changes in the measured AHE in uniaxial crystals.

We calculated the AHC in ordered FePt alloys (Fig. 2), where the presence of the heavy Pt ions induces a strong SOI. We first considered the lowest-energy ground state configuration, with the spontaneous magnetization pointing along the [001] easy-axis direction. We then recalculated the AHC with the magnetization along [100], finding that it was reduced by a factor of two. In order to understand the origin of this large anisotropy, we redid the calculations after selectively turning off the spin-flip and spin-conserving parts of the SOI. The surprising result was that the anisotropy is caused mainly by the spin-flip part of the SOI, while the spin-conserving part leads to an almost perfectly isotropic Hall effect.

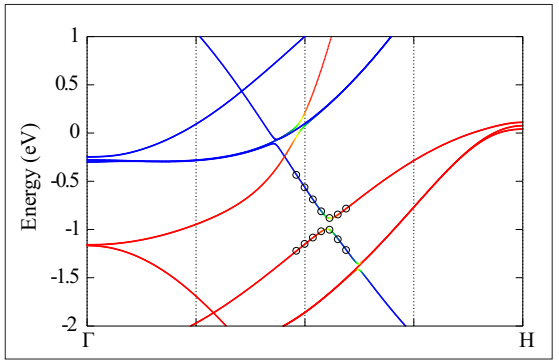


Figure 1. In the absence of spin-orbit, the energy bands in a ferromagnet (here, bcc Fe) can be classified as purely up-spin (blue) or down-spin (red). The spin-orbit interaction mixes the up- and down-spin states, leading to the rainbow-colored states with intermediate values of the spin projection along the quantization axis.

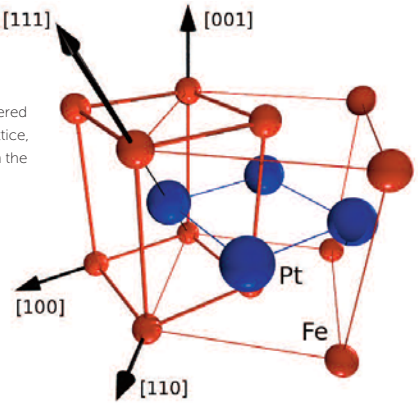


Figure 2. The uniaxial crystal structure of the ordered FePt alloy. The atoms form a face-centred cubic lattice, with alternating layers of Fe and Pt atoms stacked in the vertical direction.

The spin-orbit mixing between up- and down-spin tates in a uniaxial ferromagnet can lead to a strong dependence of the anomalous Hall conductivity on the magnetization direction.

Dye sensitized ZnO solar cells: attachment of a protoporphyrin dye to different crystal surfaces characterized by NEXAFS

R. González-Moreno, P.L. Cook, I. Zegkinoglou, X. Liu, P.S. Johnson, W. Yang,
R.E. Ruther, R.J. Hamers, R. Tena-Zaera, F.J. Himpsel, J.E. Ortega, and C. Rogero
The Journal of Physical Chemistry C. 115, 18195 (2011)

In this work, element-specific spectroscopy, particularly Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy, is used to investigate the chemistry and electronic structure at the interface between dye molecules and the ZnO acceptor electrode for dye-sensitized solar cell applications.

Dye sensitized solar cells are becoming a serious contender for low-cost solar cells. To improve their efficiency it is necessary to find the optimal combination of organic dyes, electrolytes and nanostructured anode materials. The best performance so far is achieved with a TiO2 nanocrystal anode sensitized by ruthenium-based organic dyes. This design exhibits high quantum efficiency due to the fast electron injection process into the oxide conduction band. An alternative is a ZnO nanorod array, which has the ideal architecture to minimize the charge carrier path while keeping a large active surface. However, in ZnO nanorod cells, the overall efficiency is poor. One possibe reason is a poor attachment of the dye to the ZnO surface.

With the aim of understanding the physical and chemical properties of dye-sensitized ZnO surfaces, we have analyzed the attachment of porphyrin molecules, such as free and metalated protoporphyrin, to the three low-index ZnO single crystal faces and to ZnO nanorod arrays, using near edge X-ray absorption fine structure (NEXAFS) spectroscopy. The selection of protoporphyrin was motivated by both the presence of carboxylic acid anchoring groups, and the structural simplicity, i.e., a planar geometry that allows structural characterization of the bonding through light polarization studies at the N 1s edge in NEXAFS.

Using this approach we have confirmed the importance of carboxylic groups in the anchoring of the molecules to the ZnO surfaces, similar to the situation on single crystals as Cu(110). By comparing results obtained for molecules with two propionic acid groups and molecules where the carboxylic acid groups have been replaced by two ester groups, the last did not immobilize on the ZnO surface (illustrated in Figure 1).

Moreover, we have found that the crystallographic orientation of the exposed ZnO face has a strong influence on the dye immobilization (illustrated in Figure 2). The O-terminated ZnO(0001) surface provides the maximum total uptake, and molecules are oriented such that the central macrocycle ring is perpendicular to the surface, as determined from the polarization dependence of NEXAFS. The non-polar Zn(10-10), which makes up the lateral facets of the nanowires, exhibits a lower uptake and much less polarization dependence. This can be interpreted as non-optimal anchoring, and could explain the poor efficiency of ZnO cells fabricated with nanowires instead of nanoparticles. Finally we determine that different chemical immobilization conditions produce etching on the ZnO surface. This could strongly affect to the efficiency of the possible organic cell device.

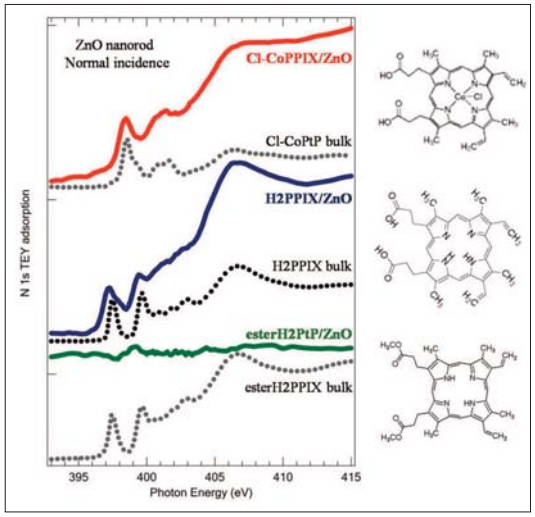


Figure 1. N1s absorption edge of different Protoporphyrin molecules attached to ZnO nanorods (full lines) compared to the molecular powders (dotted lines). Protoporphyrin dimethyl ester (esterH2PPIX) on ZnO is almost not distinguished, demonstrating the need of carboxylic groups for attaching molecules to ZnO efficiently.

ZnO nanorod arrays are desirable for organic photovoltaic devices because of the high crystallinity and the optimum architecture.

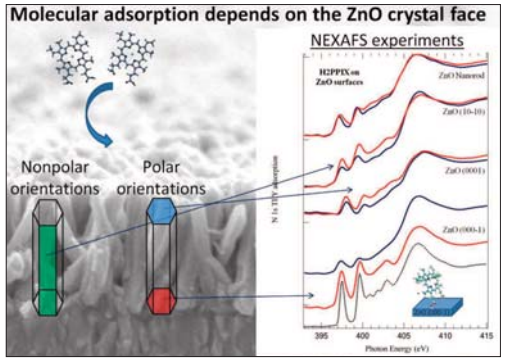


Figure 2 cross section SEM micrographs of the ZnO nanorods showing a dense array of roughly hexagonal columns. Polarization-dependent N 1s absorption edges of H2-Protoporphyrin IX on the three low-index ZnO single crystal surfaces and for ZnO nanorods. Red lines are for a polarization parallel to the surface and blue lines for mixed polarization. The (nominally) oxygen-terminated ZnO(000-1) surface exhibits the strongest polarization dependence and the highest coverage. Inserted is an illustration of the configuration of the molecule standing upright on the ZnO (000-1) surface.

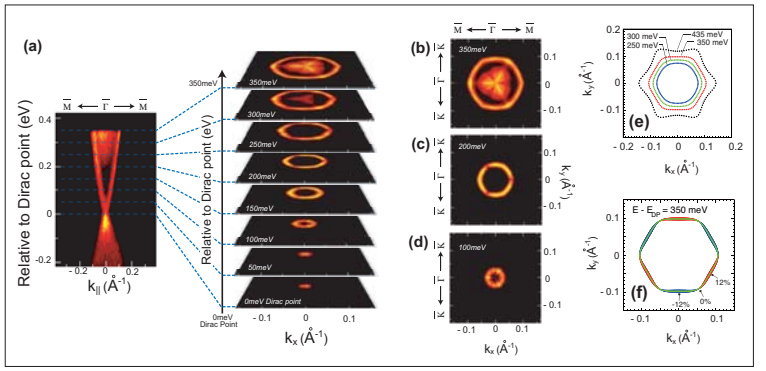
Hexagonally deformed Fermi surface of the 3D topological insulator Bi_2Se_3

K. Kuroda, M. Arita, K. Miyamoto, M. Ye, J. Jiang, A. Kimura, E.E. Krasovskii, E.V. Chulkov, H. Iwasawa, T. Okuda, K. Shimada, Y. Ueda, H. Namatame, and M. Taniguchi
Physical Review Letters 105, 076802 (2010)

A hexagonal deformation of the Fermi surface of the topological insulator Bi_2Se_3 is observed by angle-resolved photoemission spectroscopy (ARPES) and explained by *ab initio* calculations. Implications for the surface state scattering by impurities are discussed.

The three-dimensional topological insulator Bi_2Se_3 possesses "topologically protected" conducting surface states with a "massless" dispersion and helical spin texture, which could be promising for the realization of spin transport without heat dissipation. Contrary to the general belief that the surface state in Bi_2Se_3 forms an ideal Dirac cone the high-resolution ARPES measurements establish a substantial hexagonal deformation of the constant energy contours of the topological state, which disappears in approaching the Dirac point (DP). The k|| slices are presented in the Figure for several energies from the DP to E_F of undoped Bi_2Se_3. The constant energy contour (CEC) is circular at 100 meV, and in going from the DP towards EF the shape of CEC evolves from a circle to a hexagon above 200 meV, where the bulk conduction band becomes enclosed inside the surface CEC as seen in the slices at 250, 300 and 350 meV. The calculations performed with the linear augmented plane waves method agree well with the experiment, and they predict that the CEC deformation is accompanied by the appearance of a surface perpendicular spin projection, which is maximal in the ΓK direction, where it reaches 12% at 350 meV, and vanishes in the ΓM line due to the mirror symmetry. The flat segments of the hexagonal Fermi surface opposite to each other along ΓK (see Figure) may enable a strong nesting, leading to spin-density waves. The calculation further predicts the CEC deformation to occur also in the unoccupied state, where the CEC turns into a hexagram at 435 meV above the DP, and the out-of-plane spin polarization increases to 17%. Thus, a scattering channel could be opened through the vertical spin component, which would generate the quasiparticle interference by a nonmagnetic impurity on the surface.

In order to realize the quantum topological transport, the Fermi level should be brought into the energy gap by doping with non-magnetic elements. However, the dopant itself could become a scattering source. In particular, an impurity with a strong spin-orbit coupling may enhance quasiparticle interference, especially at large momenta. To minimize this effect, a light element should be chosen. This work demonstrates that by replacing 1% of Bi atoms with Mg the Fermi energy of naturally electron doped Bi_2Se_3 is brought to the Dirac point. This opens a way to the realization of the quantum topological transport regime in Bi_2Se_3 .



a) Energy dispersion curve along ΓM direction (left) and constant energy contours at several energies from 0 (Dirac point) to 350 meV (Fermi surface). CECs at (b) 100, (c) 200 and (d) 350 meV. (e) Calculated CECs at 250, 300, 350 and 435 meV for a slab of five formula units. (f) Predicted surface perpendicular projection of spin polarization for the CEC at 350 meV.

Time-dependent electron phenomena at surfaces

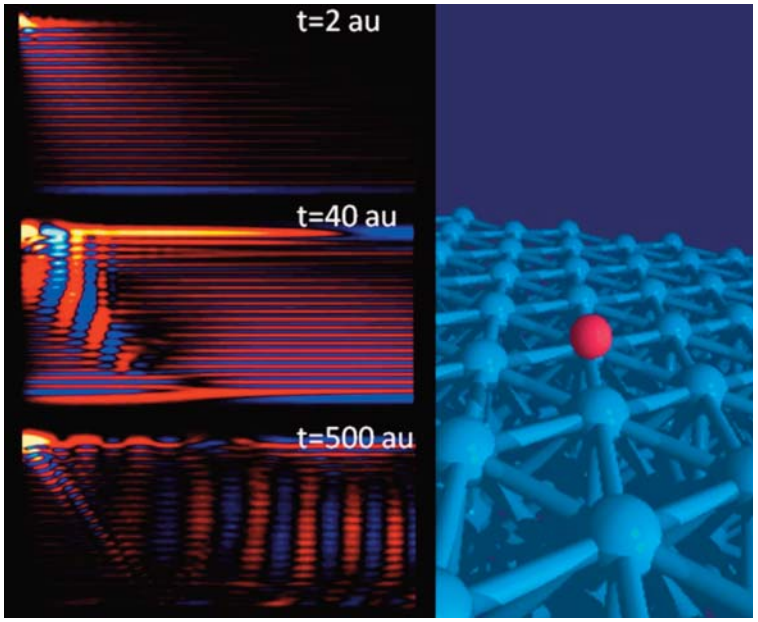
R. Díez Muiño, D. Sánchez-Portal, V.M. Silkin, E.V. Chulkov, and P.M. Echenique
Proceedings of the National Academy of Science PNAS 108, 971 (2011)

The research work summarized in the article provides new insight into the physical phenomena that appear in very small systems, in the nanometer scale, and very short times, in the attosecond scale.

In the last decade and due to the development of sophisticated experimental techniques, mostly based on laser sources, electron dynamics in nanometer-scale regions has become accessible and reasonably well understood. However, these techniques were unable to obtain time resolutions below the femtosecond scale until very recently. In practice, this limitation meant that electron dynamics could not be studied in the time scale in which chemical reactions actually happen. Ultrashort laser pulses have dramatically change the situation and attosecond physics is currently becoming a reality. Nowadays, it is indeed possible to reach the time scale in which a chemical reaction is produced or an electron is photoemitted from a surface or a nanostructure. The understanding and control of charge transfer times and electronic excitation survival times is a necessary step to understand, control, and design physical and chemical processes at surfaces. This is the focus of the scientific article published by DIPC researchers in PNAS.

In the research work summarized in the article, the authors use state-of-the-art theoretical methods to analyze very refined features of femtosecond and attosecond electron dynamics. In particular, it is shown that the screening of localized charges at metal surfaces is created locally in the attosecond time scale, while collective excitations transfer the perturbation to larger distances in longer time scales. The time necessary for an electron to jump from an adsorbed atom to a magnetic surface is also analyzed. It is predicted that the elastic width of the resonance in excited alkali adsorbates on ferromagnetic surfaces can depend on spin orientation in a counterintuitive way. Active manipulation and control of magnetic ordering down to a single atomic magnet, such as a single atomic spin on a surface, is of great importance for potential applications in spintronics. Finally, the electron–electron and electron–phonon contributions to the electronic excited states widths in ultrathin metal layers are quantitatively evaluated. The time that an electron spends traveling inside an ultrathin Pb film without suffering a collision with other electrons is found to depend on the film thickness. Increasing the thickness of an ultrathin Pb film by just one atomic layer can reduce the travelling time of electrons before collision. However, increasing the thickness of the film by two atomic layers can considerably increase this travelling time.

In summary, the study provides new insight into the physical phenomena that appear in very small systems, in the nanometer scale, and very short times, in the attosecond scale. It shows that some of the properties found in ultrafast processes at the nanoscale are far from intuitive. An additional conclusion that can be extracted from this research work is that confinement and spin effects are key factors in the behavior of electron dynamics at metal surfaces.



Time evolution of the change in electronic density induced by an external point charge at a Cu surface.

Confinement and spin effects are key factors in the behavior of electron dynamics at metal surfaces.

Plasmonic nickel antennas

J. Chen, P. Albella, Z. Pirzadeh, P. Alonso-Gonzalez, F. Huth, S. Bonetti, V. Bonanni, J. Akerman, J. Nogues, P. Vavassori, A. Dmitriev, J. Aizpurua, and R. Hillenbrand
Small 7, 2341-2347 (2011)

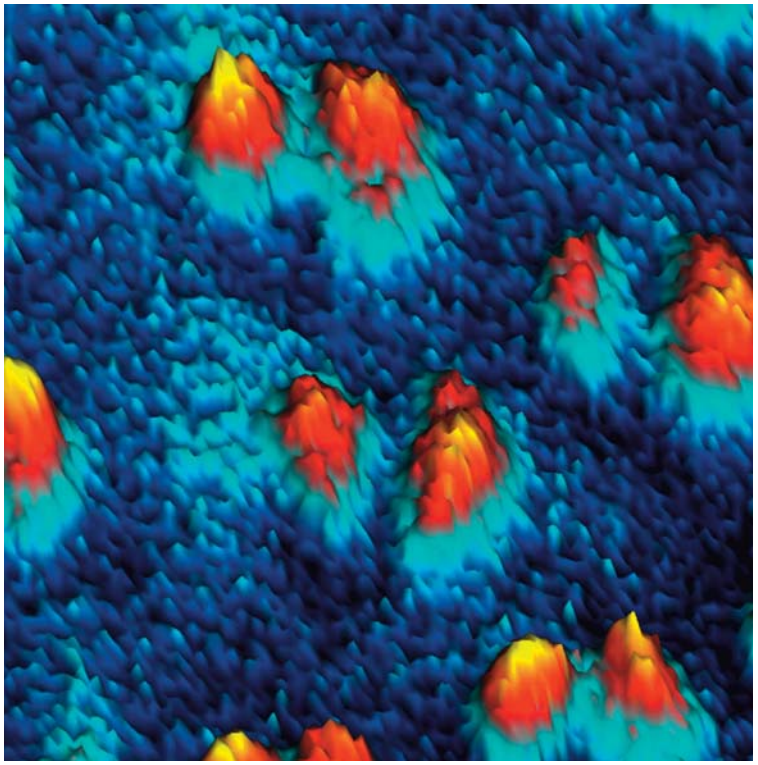
Plasmonic antennas are commonly implemented with use of gold or silver as materials, but many other materials can also perform as good field enhancers in spite of the large energy losses associated with them. In this work the fundamental optical properties of pure nickel nanoantennas are studied as a step towards understanding and engineering magnetically controllable optical nanoantennas. This novel material can be extremely useful for many developing technologies including biosensors, lasers, and solar cells.

The authors have studied the fundamental optical properties of pure nickel nanostructures by far-field extinction spectroscopy and optical near-field microscopy, providing direct experimental evidence of the existence of particle plasmon resonances predicted by theory. The synthesis of the Ni nanoantennas and the far-field optical characterization has been developed in Göteborg, Sweden, at Chalmers University of Technology, whereas the near-field characterization has been done with use of a scattering-type near-field optical microscope (s-SNOM) at the center for NanoScience and Nanotechnology nanoGUNE in San Sebastián. Researchers at DIPC have described theoretically the near-field and far-field response of the Ni antennas by means of full electrodynamical calculations. A comparison of the experimental and calculated near-field maps allow for unambiguous identification of dipolar plasmon modes in the Ni nanoparticles. Near-field images of the dipolar plasmonic modes are shown in the figure.

Furthermore, by comparing the calculated near-field and the far-field spectra, dramatic shifts between the near-field and far-field plasmon resonance are found. These shifts are more pronounced than in typical gold nanoantennas. Based on a simple damped harmonic oscillator model to describe plasmonic resonances, it is possible to explain these shifts as due to plasmon damping. Ni nanoantennas are thus identified as good platforms to reveal the spectral shifts due to their relatively large damping.

Ni nanoparticles can perform as plasmonic nanoantennas.

Shift between the spectral response of the Near-field and the Far-field identified as due to the large damping.



Near-field amplitude of Ni nanodisks acting as plasmonic antennas. The diameter of the disks is 90 nm. The dipolar mode is excited in several disks resonantly at a wavelength of 633 nm.

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Surfactant effect of sulfuric acid on the exfoliation of bilayer graphene.
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Physical Review B 84, 165424 (2011).

Extremely confined quantum-well states for (2 x 2)-K and (v3 xv3)-K on graphite: first-principles calculations.
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Physical Review B 84, 165449 (2011).

Vibrationally induced flip motion of a hydroxyl dimer on Cu(110) .
Ootsuka Y, Frederiksen T, Ueba H, and Paulsson M.
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Attosecond spectroscopy of solids: Streaking phase shift due to lattice scattering.
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Controlling the optics of quantum dots with nanomechanical strain.
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Strong electronic correlation in the hydrogen chain: A variational Monte Carlo study.
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Physical Review B 84, 245117 (2011).

Quantum-beat spectroscopy of image-potential resonances.
Marks M, Schwalb CH, Schubert K, Güdde J, and Höfer U.
Physical Review B 84, 245402 (2011).

Effect of photoelectron mean free path on the photoemission cross-section of Cu(111)
and Ag(111) Shockley states.
Lobo-Checa J, Ortega JE, Mascaraque A, Michel EG, and Krasovskii EE.
Physical Review B 84, 245419 (2011).

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Detection of ultrafast oscillations in superconducting point contacts by means of supercurrent measurements.
Avriller R , Bergeret FS, and Pistolesi F.
Physical Review B, 195415 (2011).

Self-limited oxide formation in Ni(111) oxidation.
Flege JI, Meyer A, Falta J, and Krasovskii E.
Physical Review B 84, 115441 (2011).

Tunable quantum dot arrays formed from self-assembled metal-organic networks.
Klappenberger F, Kuhne D, Krenner W, Silanes I, Arnau A, de Abajo FJG, Klyatskaya S, Ruben M, and Barth JV.
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Role of spin-flip transitions in the anomalous hall effect of FePt alloy.
Zhang HB, Freimuth F, Blugel S, Mokrousov Y, and Souza I.
Physical Review Letters 106, 117202 (2011).

Anharmonic stabilization of the high-pressure simple cubic phase of calcium.
Errea I, Rousseau B, and Bergara A.
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Role of dispersion forces in the structure of graphene monolayers on Ru surfaces.
Stradi D, Barja S, Diaz C, Garnica M, Borca B, Hinarejos JJ, Sanchez-Portal D, Alcami M, Arnau A,
de Parga ALV, Miranda R, and Martin F.
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the Cu(111) surface".
Zugarramurdi A, Zabala N, Borisov AG, and Chulkov EV.
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Spectrally resolved maker fringes in high-order harmonic generation.
Heyl CM, Güdde J, Höfer U, and L'Huillier A.
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Surface scattering via bulk continuum states in the 3D topological insulator Bi(2)Se(3).
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Shimada K, Namatame H, Taniguchi M, and Kimura A.
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Abd El-Fattah ZM, Matena M, Corso M, de Abajo, FJG, Schiller F, and Ortega JE.
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Mode-Selected electron-phonon coupling in superconducting Pb nanofilms determined from He atom scattering.
Sklyadneva IY, Benedek G, Chulkov EV, Echenique PM, Heid R, Bohnen KP, and Toennies JP.
Physical Review Letters 107, 095502 (2011).

Valence electron photoemission spectrum of semiconductors: Ab initio description of multiple satellites.
Guzzo M, Lani G, Sottile F, Romaniello P, Gatti M, Kas JJ, Rehr JJ, Silly MG, Sirotti F, and Reining L.
Physical Review Letters 107, 166401 (2011).

Quasiparticle interference around a magnetic impurity on a surface with strong spin-orbit coupling.
Strózecka A, Eiguren A, and Pascual JI.
Physical Review Letters 107, 186805 (2011).

Trapping of Image-Potential Resonances on a Free-Electron-like Surface.
Winter M, Chulkov EV, and Höfer U.
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Engineering negative differential conductance with the Cu(111) surface state.
Heinrich BW, Rastei, Choi, DJ, Frederiksen T, and Limot L.
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Circular dichroism in laser-assisted short-pulse photoionization.
Kazansky AK, Grigorieva AV, and Kabachnik.
Physical Review Letters 107, 253002 (2011).

Dynamical theory of superfluidity in one dimension.
Eggel T, Cazalilla MA, and Oshikawa M.
Physical Review Letters 107, 275302 (2011).

Proposed relationship between the exponents gamma and eta at liquid-vapour critical point via the dimensionality d.
Zhang ZD, and March NH.
Physics and Chemistry of Liquids 49, 270 (2011).

Refined semi-empirical formula for liquied-vapour critical point exponent delta and its relevance to the random field Ising model.
Zhang ZD, and March NH.
Physics and Chemistry of Liquids 49, 684, (2011).

Contribution of phonons to the line width of surface electronic states on Pd(111).
Sklyadneva IY, Tsirkin SS, Eremeev SV, Heid R, Bohnen KP, and Chulkov EV.
Physics of the Solid State 53, 2508 (2011).

Time-dependent electron phenomena at surfaces.
Diez Muiño R, Sánchez -Portal D, Silkin VM, Chulkov EV, and Echenique P.M.
PNAS 108, 971 (2011).

One dimensional bosons: From condensed matter systems to ultracold gases.
Cazalilla MA, Citro R, Giamarchi T, Orignac and Rigol M.
Reviews of Modern Physics 83, 1405 (2011).

Chlorine adsorption on the InAs (001) surface.
Bakulin AV, Eremeev SV, Tereshchenko OE, and Kulkova SE.
Semiconductors 45, 21 (2011).

Plasmonic Nickel Nanoantennas.
Chen J, Albella P, Pirzadeh Z, Alonso-Gonzalez P, Huth F, Bonetti S, Bonanni V, Akerman J, Nogues J, Vavassori P, Dmitriev A, Aizpurua J, and Hillenbrand R.
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International Soft Matter Conference 2010
Colmenero J, Richter D, and Hidalgo-Alvarez R.
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Chain dynamics in nonentangled polymer melts: A first-principle approach for the role of intramolecular barriers.
Bernabei M, Moreno AJ, Zaccarelli E, Sciortino F, and Colmenero J.
Soft Matter 7, 1364 (2011).

Structural and thermodynamic aspects of the cylinder-to-sphere transition in amphiphilic diblock copolymer micelles.
Lund R, Pipich V, Willner L, Radulescu A, Colmenero J, and Richter D.
Soft Matter 7, 1491 (2011).

Polymers under extreme two-dimensional confinement: Poly(ethylene oxide) in graphite oxide.
Barroso-Bujans F, Fernandez-Alonso F, Cerveny S, Parker SF, Alegria A, and Colmenero J.
Soft Matter 7, 7173 (2011).

Influence of surface electronic structure on the Casimir force.
Marusic L, Despoja V, Sunjic M.
Solid State Communications 151, 19 1363 (2011).

Modeling ZnS and ZnO nanostructures: structural, electronic, and optical properties.
Azpiroz JM, Mosconi E, and De Angelis F.
The Journal of Physical Chemistry C 115, 25219 (2011).

Computational evaluation of pK(a) for oxygenated side chain containing amino acids interacting with aluminum.
Mujika JI, Ugalde JM, and Lopez X.
Theoretical Chemistry Accounts 128, 477 (2011).

How accurate are electronic structure methods for actinoid chemistry?
Averkiev BB, Mantina M, Valero R, Infante I, Kovacs A, Truhlar DG, and Gagliardi L.
Theoretical Chemistry Accounts 129, 657 (2011).

Revisiting the effects of organic solvents on the thermal reduction of graphite oxide.
Barroso-Bujans F, Fierro JLG, Alegria A, and Colmenero J.
Thermochicima Acta 526, 65 (2011).

Broadband nanodielectric spectroscopy by means of amplitude modulation electrostatic force microscopy (AM-EFM).
Schwartz GA, Riedel C, Arinero R, Tordjeman P, Alegria A, and Colmenero J.
Ultramicroscopy 111, 1366 (2011).

Apertureless near-field optical microscopy: Differences between heterodyne interferometric and non-interferometric images.
Esteban R, Vogelgesang R, and Kern K.
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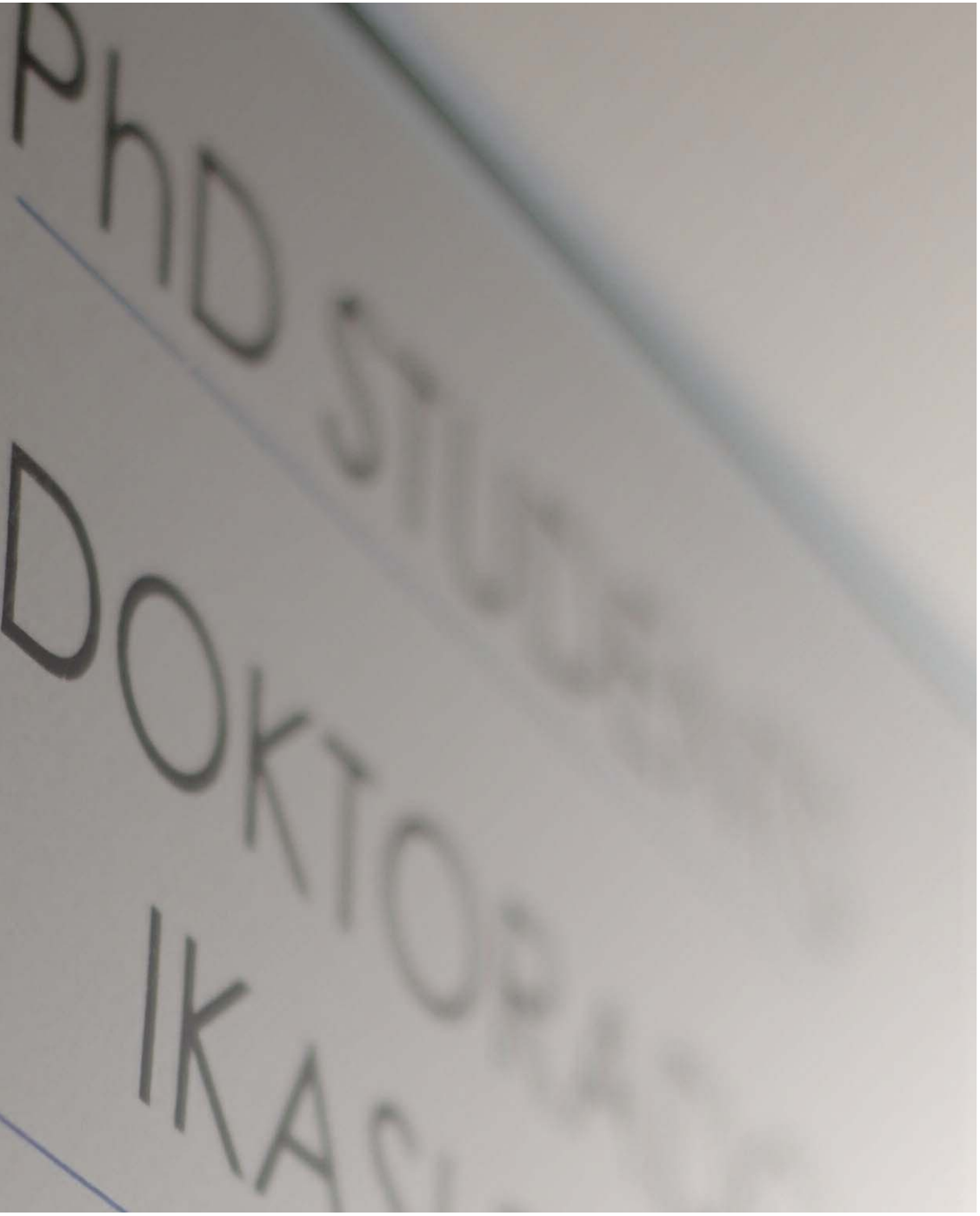


Researchers

Fellows Gipuzkoa

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

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

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

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

Dr. Maria Blanco Rey
University of Cambridge, United Kingdom
01/12/2010–Present
Metal oxide surface chemistry with applications in catalysis and physical properties of intrinsically chiral surfaces.

Postdoctoral Positions

Dr. Reidar Lund
IFF-FZ, Forschungszentrum Jülich, Germany
20/02/2006–15/10/2011
Dynamics in funcionalized polymers.

Dr. Dimas Garcia de Oteyza Feldermann
Max Planck Institute for Intelligent Systems, Stuttgart, Germany
01/09/2007–30/09/2010
The scientific work will be focused on the development of atomic force microscopy instrumentation for dielectric and conductivity measurements, in particular in polymers and semiconducting oligomers. The work will be further complemented by absorption and photoemission experiments.

Dr. Emil Lezak
Polish Academy of Sciences, Lodz, Poland
02/09/2007–31/05/2010
Plastic deformation of gamma phase isotactic polypropilene in the plane-strain compression.

Dr. Dusan Racko
Polymer Institute, SAS, Slovak Republic
03/09/2007–31/08/2010
Molecular dynamics simulations in polymers.

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

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

Dr. Virginie Boucher
École Nationale Supérieure de Chimie de Lille, France
30/10/2008–31/10/2011
Dynamical properties at molecular scale in polymeric materials multi-component and/or nano-structured combining different experimental techniques, in particular, dielectric and mechanical spectroscopy. The possibility of using x-rays and neutron scattering is also envisaged.

Dr. Remi Busselez
Universite de Rennes, France
03/11/2008–30/09/2010
The work will be focus on the study of dynamics at atomic and molecular scale in two-component polymeric systems with dynamic asymmetry by quasielastic neutron scattering and fully atomistic molecular dynamics simulations.

Dr. Ludovic Martin-Gronde
Université Bordeaux 1, France
01/09/2009–31/10/2011
Theory of elementary reactive processes at metal surfaces: Calculation of potential energy surfaces from first-principles and evaluation of reaction rates in Eley-Rideal processes.

Dr. Lokendra Pratap Singh
Jawaharlal Nehru University, New Delhi, India
07/09/2009–31/07/2011
Extend the dielectric investigation on the dynamics of the systems in higher frequencies and to compare the results with those obtained by other techniques accessing the same frequency range, namely neutron scattering and molecular dynamic simulations.

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

Dr. Manfred Matena
Universität Basel, Switzerland
01/11/2009–31-08-2011
Angle-resolved photoemission spectroscopy as well as scanning tunneling microscopy (STM) and spectroscopy (STS) are intended to be used for experimental studies on electronic and structural properties of molecular surface assemblies.

Dr. Maia García Vergniory
Lawrence Berkeley National Laboratory, USA
01/01/2010–31-12-2011
First-principles calculations of contact effect on quantum transport.

Dr. Mario Piris Silvera
UPV/EHU, Spain
01/01/2010–31/12/2010
Further development of PNOF natural orbital functional.

Dr. Duncan J. Mowbray
Center for Atomicscale Materials Design, Technical University of Denmark, Denmark
09/04/2010–31-3-2011
Time-resolved oxyde mediated photocatalisis.

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

Dr. Remi Avriller
Universidad Autónoma de Madrid, Spain
06/10/2010–30/09/2011
Inelastic quantum transport properties of nanoscale objects.

Dr. Paulina Gonzalez-Morelos
Cornell University, New York, USA
25/10/2010–31/12/2010
TDDFT study of the energy loss of swift ions in solids.

Dr. Ester Sola Badia
University College London, United Kingdom
03/11/2010–27/03/2011
Ab initio study of the structural, electronic and optical properties of nanoparticle-filled molecular cages.

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

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

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

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

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

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

Temporary Contract Position

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

Dr. Andrey Kazanskiy
University of San Petersburg, Russia
17/07/2009–31/07/2010
Electron dynamics at adsorbates on metals. Study of electron ejection from different bands of metal by attosecond pulses has been continued. Ionization of an alkali atom adsorbed on a metal surface by attosecond pulse within a streaking scheme has been considered. A computational code for study Auger ionization by attosecond pulse within the streaking scheme has been developed. A study of interaction of an electron ionized from an inner shell of an adsorbed atom with its dynamically formed image charge is in progress.

Dr. José Alfonso Pomposo Alonso
CIDETEC, Donostia-San Sebastián, Spain
16/11/2009–31/08/2010
Dynamics and Relaxation Times in Soft Nanomaterials. Our main goal is to explore the dynamics in soft nanocomposites (i.e. nanomaterials involving soft nanoparticles dispersed in a polymeric matrix) and to determine reliable relaxation times in these systems by means of broadband dielectric spectroscopy and small angle neutron scattering techniques. Theoretical models are combined with computer simulations to understand the observed experimental behaviour with special emphasis in new nanoscale effects.

PhD Students

Sara Capponi
University of Perugia, Italy
23/10/2005–30/06/2011
Dynamics of DNA and proteins by neutron scattering.

Olalla Pérez González
Facultad de Ciencia y Tecnología, UPV/EHU, Spain
02/10/2006–Present
Plasmon excitations in metallic nanoparticles. Optical properties of nanostructured materials.

Clément Riedel
Université Montpellier 2, France
05/09/2007–09/09/2011
Multiscale study of the dielectrics properties of matter from the nanoscopic scale to the macroscopic scale.

Nicolas Large
Université Paul Sabatier, Toulouse, France
01/10/2007–31/10/2011
Interaction of localized plasmons and acoustic vibrations in metallic nanostructures.

Sandra Plaza García
UPV/EHU, Spain
01/10/2007–31/12/2011
Dynamics of funtionalized polymers. Polymer functionalization is a promising tool for the development of future polymer applications. We want to know how functionalization modifies the matrix properties which is in connection with the technological application of functionalized polymers.

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

Carlos Etxeberria Arrondo
Universidad Pública de Navarra, Spain
01/01/2008–31/03/2010
Quantum dots based on magnetic semiconductors.

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

Roberto Pérez Aparicio
Universidad de Valladolid, Spain
01/09/2009–31/07/2010
Study of molecular dynamics in glass forming polymers by means of neutron scattering techniques and molecular dynamics simulations. In particular, this work focuses on the poly (ethylene propylene) (PEP) in order to study its molecular dynamics at local scales (atomic motions), large scales (chain dynamics), and also the crossover between them.

Asier Ozaeta Rodriguez
UPV/EHU, Spain
01/12/2009–30/09/2010
Transport properties of superconducting weak links in the presence of a rf-field.

Irma Pérez Baena
UPV/EHU, Spain
08/03–31/08/2010
Dynamics and phase diagrams for soft nanoparticles and all-polymer nanocomposites thereof.

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

Elixabete Goiri Little
UPV/EHU, Spain
01/07/2010–Present
Tunneling microscopy and spectroscopy of molecules on metals at 1 K.

Natalia Koval
Adyghe State University, Russia
15/07–30/09/2010
Interacción entre pequeñas moléculas y superficies metálicas: reactividad y contribuciones no adiabáticas.

Alison Crawford Uranga
UPV/EHU, Spain
01/08/2010–31/12/2011
Non.adiabatic effects in the electronic and ionic response of molecules within the time-dependent density functional theory: development of new exchange and correlation functionals.

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

Elton José Gomes dos Santos
CFM-CSIC, San Sebastián, Spain
01/01–21/10/2011
First-principles study of the electronic and magnetic properties of functionalized carbon nanostructures.

Alexander Correa Aristizabal
Universidad del Valle, Cali, Colombia
21/6/2011–Present
Studies at the nanoscale of interfaces for biosensor and solar cell applications.

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

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

Visiting Researchers

Long visits

Dr. Jianing Chen
Institute of Physics,
Chinese Academy of Sciences, China
07/01–07/02/2010
Field-enhanced Raman spectroscopy.

Dr. Svetlana Borisova
Institute of Strength Physics and Material Science,
Russian Academy of Sciences, Tomsk, Russia
26/02–26/04/2010
Phonones in metal adlayers.

Prof. Alberto Galindo Tixaire
Universidad Complutense de Madrid, Spain
10/02–10/3/2010
Quantum information and quantum algorithms. Basic problems in quantum physics. Completion of a two-volume textbook on advanced quantum mechanics, and a textbook on space-time structure.

Dr. Yury Koroteev
Tomsk State University, Russia
26/02–26/04/2010, 15/10–15/12/2010,
21/04–22/06/2011
First principles calculations of electronic structure and quasiparticle lifetimes in metals.

Prof. Wolfgang Schattke
Universität Kiel, Germany
01/03–01/04/2010, 01/06–28/07/2011
Variational Quantum Montecarlo calculations of the electronic properties of solids and surfaces. Theory of photoemission in semiconductors and metals.

Dr. Jon Otegui De La Fuente
Universidad Complutense de Madrid, Spain
10/03–31/05/2010
Bulk and surface chain dynamics under external constrains.

Prof. Vladimir Menshov
Russian Research Center "Kurchatov Institute",
Moscow, Russia
21/03–20/05/2010
Confling mechanisms in digital alloys.

Dr. Pablo Albella
Universidad de Cantabria, Spain
01/04–01/05/2010
Calculations of antenna field enhancement.

Prof. Sergio Caprara
University of Rome Sapienza and
Instituto Nazionale per la Fisica della Materia, Italy
07/04–29/05/2010, 28/02–22/04/2011
Digital alloys.

Dr. Stepan Tsirkin
Tomsk State University, Russia
08/04–06/07/2010, 04/05–29/07/2011, 16/11/2011
13/02/2012
Electronic excitations on metal surfaces, topological insulators.

Prof. Norman March
University of Antwerpen, Belgium
15/04–13/06/2010, 11/04–11/06/2011
Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

Doctorand Mikhail Otrokov
Tomsk State University, Russia
26/04–26/05/2010
Electronic structure of digital alloys.

Dr. Fernando Ruipérez Cillán
Stockholm University, AlbaNova University Centre,
Stockholm, Sweden
05/05/2010–31/07/2010
Quantum chemical study of lanthanide and actinide impurities in ionic crystals.

Dr. Alejandro Miccio
Facultad de Ingeniería - INTEMA,
Mar del Plata, Argentina
20/05–20/06/2010, 01/10–21/11/2010,
23/04–20/07/2011
Study of the fluorine concentration gradient in DGEBA samples by means of EFM. Local Dielectric Spectroscopy by means of AFM.

Dr. Maria Blanco Rey
University of Cambridge, United Kingdom
23/05/2010–25/06/2010
Metal oxide surface chemistry with applications in catalysis and physical properties of intrinsically chiral surfaces.

Dr. Arthur Ernst
Max Planck Institute of Microstructure Physics,
Halle, Germany
01/06/2010–30/06/2010
Magnetism from first principles: a multiple scattering approach.

Prof. Istvan Nagy
Technical University of Budapest, Hungary
01/06–30/06/2010
Various aspects of correlations in extended fermionic systems; spice-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Prof. Juan José Sáenz Gutiérrez
Universidad Autónoma de Madrid, Spain
01/06–31/07/2010, 01/05–31/07/2011
Nanophotonics. Modeling scanning probe microscopies.

Prof. Nikolay Kabachnik
Institut fur Experimentalphysik, Hamburg, Germany
01/06–31/07/2010, 01/06–30/08/2011
Study of Auger processes in gases and at solid surfaces within an attosecond streaking scheme.

Dr. Peter Koval
CPMOH, Université de Bordeaux, France
06/06–31/08/2010
Extension of the LCAO method SIESTA to excited states: application to organic solar cells.

Doctorand Tatiana Menshchikova
Tomsk State University, Russia
01/07–30/09/2010, 16/06–30/08/2011
Excitations on surfaces with defects.

Dr. Nicolay Zaytsev
Ufa State Aviation Technical University,
Russian Federation, Russia
01/07–31/08/2010, 07/11/2011–04/01/2012
First principle electronic structure calculations of organic molecules absorbed on metallic surfaces.

Dr. Sergey Eremeev
Institute of Strenght Physics and Materials Sciences,
Tomsk, Russia
01/07–30/09/2010, 02/06–31/08/2011
Phonons and electron-phonon coupling in quantum-well states of adlayers on metals.
Electronic properties of topological insulators.

Prof. Mario Trioni
CNR, University of Milano-Bicocca, Italy
01/07–31/07/2010
Electronic and magnetic properties of thin solid film on metals.

Dr. Ilya Nechaev
Kostroma State University, Russia
15/07–15/08/2010, 01/07–27/09/2011
Electron excitations in ferromagnetic materials

Prof. Julio Alonso Martín
Universidad de Valladolid, Spain
20/07–20/08/2010
Computational simulation of the intercalation of alkaline atoms in graphite and carbon nanotubes.
Laser induced fragmentation of atomic clusters.

Prof. Amand Lucas
FUNDP, Namur, Belgium
03/08–31/10/2010, 02/08–30/10/2011
Condensed matter physics, surface sciences, electronic and atomic structures of reduced dimensionality systems structural biology.

Prof. Vladimir Kuznetsov
Tomsk State University, Russia
08/08–10/09/2010, 07/08–08/09/2011
Density functional methods in the theory of phase diagrams of alloys and in the Kondo effects.

Prof. Wlodzimierz Jaskólski
Institute of Physics, Nicholas Copernicus University, Poland
01/09–30/09/2010
Study of quantum dot arrays and nanotube superlattices.

Prof. Marijan Sunjic
University of Zagreb, Croatia
06/09–28/10/2010, 01/02–26/02/2011,
01/09–30/10/2011
Dynamical response and surface excitations in thin films.

Dr. Galina Rusina
Russian Academy of Sciences, Tomsk, Russia
31/10/2010–30/01/2011, 01/11/2011–31/01/2012
Surface phonons in CuPd surface alloys.

Dr. Andrey Vasenko
LPMMC, Université Joseph Fourier and CNRS, Grenoble, France
01/11/2010–22/12/2010
Electron cooling by diffusive ferromagnetic metal - superconductor junctions.

Dr. Ivo Souza
University of Berkeley, USA
06/01–06/02/2011
Theory of polarization and orbital magnetization in condensed matter.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Italy
10/01–28/02/2011, 07/09–31/10/2011
Surface phonons and phase transitions.

Prof. Victor Tugushev
Russian Research Center "Kurchatov Institute", Moscow, Russia
11/01–07/04/2011
Magnetism in superlattices and spintronics.

Doctorand Andrey Kuznetsov
Tomsk State University, Russia
15/01–15/02/2011, 04/09–03/11/2011
Magnetic effects on the formation of defects in bulk Fe and in thin Fe films.

Prof. Andrey Kazanskiy
University of San Petersburg, Russia
16/01–28/02/2011
Electron dynamics at adsorbates on metals.

Dr. Imamaddin Amiraslanov
Institute of Physics, ANAS, Baku, Azerbaijan
01/02–01/03/2011
Thermoelectric materials growth and crystal structures.

Dr. Ziya Aliyev
Baku State University, Azerbaijan
01/02–26/04/2011
Materials physics of topological insulators.

Dr. Iñigo Garcia Yoldi
Instituto de Ciencia y Tecnología de Polimeros, CSIC Madrid, Spain
01/02–28/02/2011
Simulation of confined polymers.

Prof. Vladlen Zhukov
Ural Branch of Russian Academy of Sciences, Ekaterinbourg, Russia
12/02–07/05/2011, 02/08–23/09/2011
Electron dynamics in oxides: electron-electron and electron-phonon mechanisms of decay of excited electrons.

Prof. Malcolm Stott
Queen's University, Kingston, Canada
01/03–31/03/2011
2D electron gas.

Dr. Miguel De Castro Vítores
Universidad Autonoma Madrid, Spain
14/03–15/06/2011
Classical reaction dynamics in quantum spirit.

Dr. Svetlana Borisova
Physics and Materials Science,
Russian Academy of Sciences, Tomsk, Russia
11/03–08/05/2011
Defects and vibrations in topological insulators.

Prof. Vladimir Menshov
Russian Research Center "Kurchatov Institute", Moscow, Russia
11/04–10/07/2011
Magnetic impurities in digital alloys and topological insulators.

Doctorand Hernan Santos-Exposito
Instituto de Ciencia de Materiales de Madrid (ICMM), Spain
01/05–31/07/2011
Graphene nanoribbons.

Dr. Li-Ming Yang
University of Oslo, Norway
01/06–31/07/2011
New materials under pressure. Analysis and characterization of their physical and chemical properties.

Prof. Wolfgang Schattke
Universität Kiel, Germany
01/06–28/07/2011
Variational Quantum Montecarlo calculations of the electronic properties of solids and surfaces. Theory of photoemission in semiconductors and metals.

Dr. Sara Pagnotta
Centro de Física de Materiales (CFM), Spain
01/06–31/07/2011
Dielectric spectroscopy measurements on water solutions of trehalose are performed and analyzed in order to understand the origin of trehalose peculiarity (with respect to other sugars) in preserving biosystem structure and function. In particular, the specific role of water dynamics is investigated.

Prof. Hannes Raebiger
Yokohama National University, Japan
03/06–03/07/2011
Diluted magnetic semiconductors.

Dr. Alejandro Reyes Coronado
Centro de Ciencias Aplicadas y Desarrollo Tecnológico, México
30/06–02/09/2011, 23/10–15/12/2011
Optical response of resonant metallic nanostructures in surface-enhanced microscopy and spectroscopy. Forces in metallic particles induced by fast electrons.

Doctorand Carlo Motta
Universitá di Milano-Bicocca, Italy
03/07–04/08/2011
Ab initio study of transport in nanojunctions: application to dye-sensitized solar cells.

Prof. Stefan Maier
Imperial College London, United Kingdom
15/07–15/08/2011
Plasmonics for sensing.

Dr. Andrea Donarini
Institute of Theoretical Physics,
University of Regensburg, Germany
01/09–15/10/2011
Transport characteristics of complex interacting nano-junctions.

Prof. Pedro Luis de Andres Rodríguez
Instituto Ciencia de Materiales de Madrid, CSIC, Spain
01/09–30/10/2011
Effect of stress in the chemical activity of graphene.

Doctorand Igor Rusinov
Tomsk State University, Russia
19/09–19/10/2011
Electronic structure of the magnetic semiconductor digital alloys.

Dr. Mikhail Otrokov
State University of Tomsk, Russia
19/09–19/11/2011
Electronic structure of the magnetic semiconductor digital alloys.

Dr. Simona Achilli
CNR Universitá di Milano-Bicocca, Italy
01/10–30/11/2011
Electronic and magnetic properties of single adatoms on metal surfaces.

Doctorand Astislav Bozhevolnov
Saint Petersburg State University, Russia
09/10–09/12/2011
Non-statonary study of Low Energy Electron Difraction and Photoionization.

Dr. Ziya Aliyev
Baku State University, Azerbaijan
23/10–20/12/2011
Materials physics of topological insulators.

Doctorand Igor Vishnevskii
Tomsk State University, Russia
01/11–03/12/2011
The electronic structure of topological insulators.

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

Dr. Debsindhu Bhowmik
Laboratoire Léon Brillouis (CEA-NRS), France
30/11–31/12/2011
Behavior of hydrophobic ions in aqueous medium.

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

Visiting Researchers

Short visits

Prof. Istvan Nagy
Technical University of Budapest, Hungary
04/01–31/01/2010, 23/08–18/09/2010,
03/01–29/01/2011, 26/04–21/05/2011,
22/08–18/09/2011
Various aspects of correlations in extended fermionic systems; spice-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Prof. Lawrence Glasser
Clarkson University, New York, USA
11/01–16/01/2010, 09/01–14/01/2011
Mathematical physics applied to condensed matter.

Prof. Yanming Ma
State Key Lab of Superhard Materials, Jilin University, Changchun, China
28/01–28/01/2010
Novel high pressure structures from first principles.

Prof. Fernando Cossío Mora
UPV/EHU, Donostia-San Sebastián, Spain
29/01–29/01/2010
Cycloaddition chemistry as a tool for the preparation of valuable molecules and materials.

Prof. Richard Arinero
Université Montpellier 2, France
31/01–03/02/2010, 21/06–24/06/2011
Dielectric spectroscopy at nano-scale by atomic force microscopy (AFM) techniques.

Doctorand Jhon Wilfer González Salazar
Instituto de Ciencia de Materiales de Madrid, Spain
07/02–13/02/2010
Electronic structure calculations in nanotubes.

Dr. Leonor Chico Gómez
Instituto de Ciencia de Materiales de Madrid, Spain
07/02–12/02/2010, 23/05–25/05/2011,
20/06–25/06/2011
Electronic structure calculations in nanotubes.

Dr. Jorge Lobo Checa
CIN2, Universidad Autónoma de Barcelona, Spain
08/02–20/02/2010, 15/06–18/06/2010
Study of the electronic structure of thin organic molecular layers on metal and semiconductor substrates.

Prof. Zhenchao Dong
Hefei National Laboratory for
Physical Sciences at the Microscale,
University of Science and Technology of China
09/02–11/02/2010
Molecular fluorescence in scanning tunneling microscopy cavities.

Dr. Juliane Loichen
Goodyear Technical Center, Luxembourg
09/02–11/02/2010, 25/01–27/01/2011
Nano-dielectric spectroscopy.

Dr. Stephan Westermann
Goodyear Technical Center, Luxembourg
09/02–11/02/2010, 25/01–27/01/2011
Nano-dielectric spectroscopy.

Prof. Marijan Sunjic
University of Zagreb, Croatia
11/02–26/02/2010
Dynamical response and surface excitations in thin films.

Dr. Simona Achilli
University of Milano-Bicocca, Italy
12/02–28/02/2010, 31/05–03/06/2011
Electronic and magnetic properties of single adatoms on metal surfaces.

Dr. Maider Machado
Fundación Inasmet, San Sebastián
12/02–12/02/2010
Building integrated photovoltaics: technology and applications.

Dr. Miguel Angel Muñoz Marqués
Instituto Ciencia de Materiales de Sevilla, Spain
14/02–15/02/2010
Surface structural studies with MEIS.

Doctorand Grethe Vestergaard
Jensen Aarhus University, Denmark
17/02–24/02/2010
Small angle x-ray scattering applied to soft condensed matter systems.

Dr. Leonardo Marusic
University of Zadar, Croatia
21/02–26/02/2010
Surface science. Casimir forces between metalic slabs. Polariton spectra.

Prof. Malcolm Stott
Queen's University, Kingston, Canada
22/02–26/02/2010
2D electron gas.

Prof. Mario Trioni
CNR, University of Milano-Bicocca, Italy
22/02–26/02/2010, 21/10–28/10/2011,
17/11–19/11/2011
Electronic and magnetic properties of thin solid film on metals.

Prof. Alexander Buzdin
Université Bourdeaux I, France
01/03–2/03/2010
Coexistence of ferromagnetism and superconductivity.

Prof. Javier Tejada Palacios
Universidad de Barcelona, Barcelona , Spain
04/03–5/03/2010
Quantum Rotational Motion in mesoscopic systems.

Dr. Pawel Rejmak
Institute of Catalysis and Surface Chemistry of Polish Academy of Science, Poland
24/03–27/03/2010
First-principles calculations on nanostructures.

Dr. Andrey Vasenko
LPMMC, Universite Joseph Fourier and CNRS, France
25/03–27/03/2010
Electron cooling by diffusive normal metal - superconductor tunnel junctions.

Dr. Marten Piantek
Freie Universitaet Berlin, Germany
09/04–9/04/2010
Switchable molecules on metallic surfaces.

Prof. Dieter Richter
IFF-FZ, Forschungszentrum Jülich, Germany
10/04–18/04/2010
Polymer dynamics by neutron techniques.

Dr. Fernando Ruipérez Cillán
Stockholm University, AlbaNova University Centre, Stockholm, Sweden
12/04–12/04/2010
Quantum chemical study of lanthanide and actinide impurities in ionic crystals.

Dr. Remi Avriller
Facultad de Ciencias, Universidad Autónoma de Madrid, Spain, CEA Grenoble and Université Joseph Fourier, France
15/04–17/04/2010
Quantum transport in nanostructures in presence of strong external perturbations.

Prof. Jean Jaques Greffet
Institut d'Optique Graduate School,
Institut Universitaire de France, Palaiseau, France
22/04–24/04/2010
Nano-optics: Theory of nanoparticle resonances from visible to THz.

Prof. Enrique Solano Villanueva
UPV/EHU, Leioa, Spain
30/04–30/04/2010
Quantum Technologies with Circuit QED.

Prof. José Luis Vicent López
Facultad CC. Físicas, Universidad Complutense,Madrid, Spain
13/05–15/05/2010
Dynamics effects in superconducting/magnetic nanostructures.

Dr. Peter Koval
CPMOH, Université de Bordeaux, France
17/05–18/05/2010
Extension of the LCAO method SIESTA to excited states: application to organic solar cells

Prof. Dietrich Foerster
CPMOH, Université de Bordeaux, France
17/05–18/05/2010, 20/04–22/04/2011,
13/07–15/07/2011, 26/07–29/07/2011
Extension of the LCAO method SIESTA to excited states: application to organic solar cells.

Dr. Daniele Stradi
Universidad Autónoma de Madrid
06/05–7/05/2010
Self-assembly and reactivity on the graphene/Ru[0001] surface.

Dr. Arthur Ernst
Max-Planck-Institut für Mikrostrukturphysik, Germany
11/05–15/05/2010
Magnetism from first principles: a multiple scattering approach.

Dr. Aaron Bostwick
Advanced Light Source, Lawrence Berkeley Lab, USA
12/05–19/05/2010
Graphene band structure with angle resolved photoemission.

Prof. James D. Talman
University of Western Ontario, Canada
12/05–26/05/2010, 10/07–17/07/2011, 24/07–30/07/2011
Efficient methods in quantum chemistry.

Prof. Bo Hellsing
Chalmers and Göteborg University, Sweden
24/05–28/05/2010
Electron-phonon interactions on metal surfaces.

Dr. Vitaly Pipich
JCNS/FRMII c/o TU Muenchen, Garching, Germany
27/05–05/06/2010
Small-angle neutron scattering applied to soft matter systems.

Prof. Garnett W. Bryant
NIST, Gaithersburg, Maryland, USA
29/05–04/06/2010
Nanophotonics

Prof. Luciano Colombo
University of Cagliari and SLACS (INFM-CNR), Italy
26/05–29/05/2010
Growth phenomena in mixed amorphous/crystalline silicon nanosystems.

Dr. Miguel Angel Gosalvez Ayuso
Nagoya University, Japan
31/05–07/06/2010
Macroscopic and microscopic kinetics in surface processing: heterogeneous catalysis, heteroepitaxial growth and anisotropic etching.

Dr. Remi Vincent
Institut Langevin Ondes et Images, CNRS - ESPCI Paris, France
03/06–20/06/2010
Study and control of fluorescence with magneto-optical nanostructures.

Dr. Sergey Ostanin
Max-Planck-Institut für Mikrostrukturphysik, Germany
07/06–13/06/2010
Magnetism from first principles: a multiple scattering approach.

Prof. Frank Hekking
Laboratoire de Physique et de Modélisation des Milieux Condensés, Université Joseph Fourier and CNRS, Grenoble, France
06/06–09/06/2010
Phase-charge duality in Josephson junction circuits: Role of inertia and effect of microwave irradiation.

Dr. Jürgen Henk
Max-Planck-Institut für Mikrostrukturphysik, Germany
08/06–11/06/2010
Ferroelectric control of Rashba spin-orbit coupling.

Prof. Pedro de Andres Rodriguez
Instituto de Ciencia de Materiales de Madrid CSIC, Spain
14/06–16/06/2010
Adsorption and diffusion of atomic and molecular hydrogen on graphene and graphite.

Prof. Avelino Corma Canós
Instituto de Tecnología Química, UPV-CSIC, Universidad Politécnica de Valencia, Spain
15/06–16/06/2010
Multifunctional materials design for catalysis.

Dr. Anders Mathias Lunde
ICMM, CSIC, Madrid, Spain
17/06–18/06/2010
Interaction induced edge channel equilibration.

Dr. Alexander Yaresko
Max-Planck-Institut für Festkörperforschung, Germany
20/06–27/06/2010, 05/09–04/010/2011
Theoretical study of x-ray absorption and magnetic circular dichroism in novel materials.

Prof. Mario Rocca Agostino
Università degli Studi di Genova, Italy
21/06–23/06/2010
Surface science spectroscopy.

Prof. Lin-Wang Wang
Lawrence Berkeley National Laboratory, USA
27/06–30/06/2010
Electronic quantum transport

Dr. Oleg Tereshchenko
Institut of Semiconductor Physics, Novosibirsk, Russia
30/06–04/07/2010
Two-dimentional plasmons and electric transport in metal layers deposited on semiconductors.

Doctorand Petra Bacova
Charles University, Czech Republic
01/07–15/07/2010
Dynamics of branching points in complex polymers.

Dr. Kiron Burke
University of California, Irvine, USA
04/07–06/07/2010
Density-Functional Theory

Dr. Martin Brodeck
Forschungszentrum Jülich GmbH, Germany
07/07–15/07/2010
MD simulations of polymers confined by walls.

Dr. Rene Gaudoin
Universität Wien, Austria
09/07–17/07/2010, 12/09–16/09/2011
Reciprocal-space finite-size corrections for Quantum Monte Carlo calculations. Diffusion Monte Carlo.

Dr. Lucian Constantin
Theoretical and Computational division of the National Nanotechnology Laboratory of CNR-INFM, Lecce, Italy
13/07–17/07/2010
Density-Functional theory.

Prof. Andrei Postnikov
Paul Verlaine Université-Metz, France
13/07–14/07/2010
Phonons in mixed semiconductors.

Dr. Mau-scheng Zei
National Central University, Taiwan
19/07–20/07/2010
Electrochemical deposition of metallic films and nanoparticles on thin oxides and metallic surfaces.

Prof. Emilio Artacho Cortés
University of Cambridge, United Kingdom
19/07–11/08/2010
Electronic stopping power in insulators. LDA+U, SIC, exact-exchange in DFT calculations.

Prof. Fernando Sols
Universidad Complutense de Madrid, Spain
21/07–23/07/2010
Electron cooling in nanostructures.

Doctorand Gregor Michalicek
Forschungszentrum Jülich GmbH, Germany
21/07–23/07/2010
Magnetic properties of low dimensional systems and nano-structures by ab initio methods.

Prof. Stefan Blügel
Forschungszentrum Jülich GmbH, Germany
21/07–23/07/2010
Magnetic properties of low dimensional systems and nano-structures by ab initio methods.

Doctorand Thomas Zinn
Forschungszentrum Jülich GmbH, Germany
23/07–03/08/2010
Chain exchange kinetics of n-alkane-PEO block copolymer micelles.

Dr. Mario Cuoco
CNR-SPIN "E.R.Caianiello", Universita di Salerno, Italy
27/07–29/07/2010
Competing broken symmetries due to magnetism and unconventional superconductivity in hybrid .structures.

Prof. Godfrey Gumbs
Hunter College, The City University of New York, USA
02/08–28/08/2010, 09/08–3/09/2011
Plasmons in nanostructures.

Doctorand Jorge Zuloaga Franco
Rice University, Texas, USA
06/08–10/08/2010
TDDFT calculation of plasmon response in metallic nanostructures.

Dr. Hugo Dil
Universität Zürich, Switzerland
18/08–23/08/2010, 17/04–19/04/2011
New developments in topological insulators and other low dimensional systems with strong spin-orbit interaction. Spin structure investigations in topological insulators.

Prof. Gustav Bihlmayer
Forschungszentrum Jülich GmbH, Germany
27/08–02/09/2010
Magnetism in low dimensions: Overlayers, wires and atoms.

Prof. Stetzer MacKenzie
University of Washington, USA
31/08–31/08/2010
New insights into student understanding of electric circuits and analog electronics.

Dr. Rajendra Singh Dhaka
Max-Planck-Institut für Mikrostrukturphysik, Germany
04/09–06/09/2010
Photoemission study of rare gas nano-bubbles in Al(111): core-levels and plasmon excitation.

Prof. Akira Ishii
Tottori University Koyama, Japan
08/09–11/09/2010
Theory of solid state physics, mainly performing calculations of new materials and processes within density functional theory. Examples of his last topics related to surfaces are (i) reconstructions in semiconductor surfaces and (ii) adatoma adsorption and migration in graphene.

Prof. Vladimir Nazarov
RCAS, Academia Sinica, Taipei, Taiwan
08/09–05/10/2010
Time-dependent density-functional theory of particle-solid interactions.

Dr. Jan Ingo Flege
Institute of Solid State Physics, University of Bremen, Germany
11/09–15/09/2010
Surface oxidation and oxidation catalysis on metal surfaces.

Doctorand Axel Meyer
Institute of Solid State Physics, University of Bremen, Germany
11/09–15/09/2010
Surface oxidation and oxidation catalysis on metal surfaces.

Prof. Juan Rojo
Universidad Complutense de Madrid, Spain
16/09/2010–17/09/2010
Surface defects: from mechanical properties to the origin of life.

Dr. Steffen Ruettinger
PicoQuant GmbH, Berlin, Germany
23/09/2010–23/09/2010
Modern approaches to time-resolved single molecule microscopy.

Prof. Roderic Quirk
The University of Akron, Ohio, USA
26/09–06/10/2010, 08/10–15/10/2011
Synthesis of functional polymers.

Dr. Alejandro Reyes Coronado
Foundation for Research & Technology - Hellas (FORTH), Institute of Electronic Structure and Laser (IESL), Crete, Greece
26/09–09/10/2010
Optical response of resonant metallic nanostructures in surface-enhanced microscopy and spectroscopy. Forces in metallic particles induced by fast electrons.

Prof. Archie Howie
Cavendish Laboratory, Cambridge, United Kingdom
26/09–10/10/2010, 01/09–14/09/2011
Theory of valence electron excitations by fast electrons.

Prof. Satoshi Koizumi
Japan Atomic Energy Agency, Ibaraki-ken, Japan
27/09–06/10/2010
Dynamical and structural features in systems with strong dynamic asymmetry.

Dr. Maria Blanco Rey
University of Cambridge, United Kingdom
27/09–08/10/2010
Metal oxide surface chemistry with applications in catalysis and physical properties of intrinsically chiral surfaces.

Dr. Otto Muskens
University of Southampton, United Kingdom
27/09–02/10/2010
Ultrafast optical switchers.

Dr. Vojislav Krstic
College Green, Trinity College Dublin, Ireland
30/09–02/10/2010
Magnetotransport in carbón nanotube-based mesoscopic systems.

Dr. Daniele Stradi
Universidad Autónoma de Madrid
01/10–23/10/2010
Self-assembly and reactivity on the graphene/Ru[0001] surface.

Prof. Valery Tyuterev
Tomsk State Pedagogical University, Toms, Russia
01/10–28/10/2010
Phonones and electron dynamics in solids.

Prof. Tadaaki Nagao
National Institute of Materials Science, Tsukuba, Japan
02/10–07/10/2010
Plasmons in atomic changes and in atomic sheets.

Prof. Branko Gumhalter
University of Zagreb, Croatia
02/10–08/10/2010
Ultrafast electron dynamics on metal surfaces.

Dr. Fabio Busnengo
Universidad de Rosario, Argentina
04/10–23/10/2010
Dissociation of diatomic molecules at surfaces.

Dr. Jörg Meyer
Fritz-Haber-Institut, Berlin
04/10–05/10/2010
Gas/surface dynamic

Prof. Artem R. Oganov
Stony Brook University, New York, USA
08/10–10/10/2010
Novel phenomena at high pressure.

Dr. Nikolai Gaponik
Technical University Dresden, Germany
17/10–19/10/2010
Strongly emitting colloidal nanocrystals and their assemblies.

Dr. Fabio Pistolesi
Université Bordeaux / CNRS, Talence, France
20/10–22/10/2010
Euler buckling instability and enhanced current blockade in suspended single-electron transistors.

Dr. Iñigo Garcia Yoldi
Instituto de Ciencia y Tecnología (CSIC) Madrid
21/10–21/10/2010
Computer simulation of molecular crystals and polymers. From abinitio methods to molecular dynamics.

Dr. Jordi Fraxedas Calduch
Centre d' Investigació en Nanociència i Nanotecnologia CIN2(CSIC-ICN)
21/10–22/10/2010
Water-solid interfaces at ambient conditions.

Prof. Dietrich Foerster
CPMOH, Université de Bordeaux, France
24/10–26/10/2010
Extension of the LCAO method SIESTA to excited states: application to organic solar cells.

Prof. Garnett W. Bryant
NIST, Gaithersburg, Maryland, USA
26/10–30/10/2010
Nanophotonics

Prof. Peter Apell
Chalmers University of Technology, Sweden
26/10–30/10/2010, 29/11–3/12/2011
Biophysics: from surfaces modes to wound healing.

Prof. Antonio Hernando Grande
Instituto de Magnetismo Aplicado, UCM-CSIC-ADIF, Madrid, Spain
02/11–04/11/2010
Magnetism in functionalized nanoparticles.

Dr. Davide Donadio
Max-Planck-Institut für Polymerforschung, Germany
08/11–12/11/2010
Thermal transport and thermoelectric materials.

Prof. Stefan Blügel
Forschungszentrum Jülich GmbH, Germany
08/11–12/11/2010
Magnetic properties of low dimensional systems and nano-structures by ab initio methods.

Dr. Blanca Arizti García
Procter & Gamble, Spain
11/11–11/11/2010
Presentation of the Procter & Gamble's PhD Seminars

Prof. Ivan Chernov
Politechnic University of Tomsk, Russia
15/11–21/11/2010
Dynamics of hydrogen in metals under external irradiation.

Prof. Pol Van Dorpe
IMEC, Leuven, Belgium
17/11–19/11/2010
Synthesis and characterisation of plasmonic devices.

Dr. Ivan Shelykh
University of Iceland, Iceland
18/11–20/11/2010
Plasmonics: integrated devices and cavities for biosensing applications.

Prof. Mahammad Babanly
Baku State University, Baku, Azerbaijan
19/11–30/11/2010
Topological insulators: materials and properties.

Prof. Félix Yndurain Muñoz
Universidad Autónoma de Madrid, Spain
21/11–04/12/2010
Magnetisem in low dimensional systems.

Doctorand Néstor Ferrando Jódar
Universidad Politécnica de Valencia
01/12–06/12/2010
Speeding up cellular automata simulations by using GPUs.

Dr. Patrizia Borghetti
Universita Cattolica del Sacro Cuore, Brescia, Italy
08/12–10/12/2010
Self-assembly and electronic properties of macromolecular systems: ordered ultrathin porphyrin layers vs hierarchically assembled eumelanin thin films.

Dr. Andrew Ho
Royal Holloway, University of London, United Kingdom
04/01–10/01/2011
Effects of disorder in one-dimensional quantum liquids, and phase diagram of binary mixtures of one-dimensional harmonic fluids, strongly correlated cold atom systems.

Dr. Giulia Rossi
Aalto University, School of Science and Technology, Helsinki, Finland
12/01–15/01/2011
Coarse-graining polymers with the MARTINI approach.

Prof. Ralph Ernstorfer
Fritz Haber Institute, Berlin, Germany
23/01–26/01/2011
Attosecond electron dynamics in solids.

Prof. Juan José Saenz Gutierrez
Universidad Autónoma de Madrid, Spain
26/01–29/01/2011
Nanophotonics. Modeling scanning probe microscopies.

Doctorand Mikolaj Kajetan Schmidt
Copernico University, Torun, Poland
31/01–18/02/2011
Nanophotonics.

Dr. Tapio Ala-Nissila
Aalto University School of Science and Technology, Helsinki, Finland
12/01–15/01/2011
Colaboration: Coarse-grained simulations of polymer systems.

Prof. Adnen Mlayah
Université Paul Savatier, Toulouse, France
31/01–01/02/2011
Plasmon and acoustic phonon coupling.

Dr. Guillermo Romero Huenchuñir
UPV/EHU, Leioa, Spain
31/01–04/02/2011
Andreev qubit in a cavity.

Dr. Alvise Verso
Ulm University, Germany
13/01–15/01/2011
Readout of a superconducting qubit: a problem of quantum escape processes for driven systems.

Dr. Guido Goracci
University of Perugia, Italy
03/02–05/02/2011
Dynamics of DNA and DNA with water in the picosecond range by neutron scattering.

Dr. Linda A. Zotti
Universidad Autónoma de Madrid, Spain
09/02–12/02/2011
The role of anchoring groups in the electrical conduction through single molecule junctions.

Doctorand Alexander Generalov
Technische Universität Dresden, Germany
02/02–16/02/2011
Scanning tunnelling microscopy and photoemission of Cobalt nanodots.

Doctorand Andrea Trabattoni
Universitá degli Studi di Milano Bicoca, Milano, Italy
07/02–12/02/2011
Trapping photons by photonic quasi-crystals.

Prof. Vladimir Hiznjakov
University of Tartu, Estonia
13/02–19/02/2011
Molecular sprectoscoy in Helium droplets.

Prof. Akio Kimura
University of Hiroshima, Japan
22/02–01/03/2011
Electronic structure and properties of topological insulators.

Prof. John Ellis
Cavendish Laboratory, University of Cambridge, United Kingdom
23/02–25/02/2011
3He spin-echo spectroscopy of surface dynamical phenomena.

Dr. Clémence Le Coeur
Laboratoire de Physique des Solides, Paris, France
24/02–25/02/2011
Influence of macromolecular crowding on protein stability.

Prof. Taichi Okuda
University of Hiroshima, Japan
22/02–01/03/2011
Electronic structure and properties of topological insulators.

Prof. Franz J. Himpsel
University of Wisconsin, USA
23/02–04/03/2011
Using synchrotron radiation to shed light on solar cells.

Prof. Dietrich Menzel
Technische Universität München and Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany
02/03–05/03/2011
Ultrafast charge transfer at graphene surfaces.

Prof. Richard O. Prum
Yale University, Peabody Museum of Natural History, Connecticut, USA
07/03–11/03/2011
Optical properties of natural structures: an evolutionist approach.

Dr. Ralph Vogelgesang
Max-Planck-Institut für Festkörperforschung, Nano-Optics, Stuttgart, Germany
10/03–11/03/2011
Study of plasmonics by means of near-field optical microsocopy.

Prof. Roderic Quirk
The University of Akron, Ohio, USA
12/03–18/03/2011
Synthesis of functional polymers.

Dr. Laurent Bonnet
Institut des Sciences Moleculaires, Université de Bordeaux I, France
16/03–18/03/2011
Classical reaction dynamics in quantum spirit.

Dr. Roberto Otero Martín
Univ. Autónoma de Madrid, Spain
18/03–18/03/2011
Structural and chemical effects of charge-transfer across metal-organic interfaces.

Dr. Alexey Kuzmenko
Université de Genève, Switzerland
22/03–25/03/2011
Optics of Graphene.

Dr. Marisa Michelini
University of Udine, Italy
23/03–23/03/2011
The methodology of research in physics education used in the university of Udine.

Prof. Maria Silvia Gravielle
Instituto de Astronomía y Física del Espacio, Universidad de Buenos Aires, Argentina
27/03–01/04/0211
Interaction of laser pulses with metallic surfaces.

Prof. Alexander Eychmüller
Technical University of Dresden, Germany
30/03–01/04/2011
Optoelectronic properties in low-dimensional systems.

Dr. Elena Bichoutskaia
University of Nottingham, United Kingdom
05/04–05/04/2011
New approach to studying the interaction between charged particles and its impact on science.

Prof. José Angel Martín Gago
Insittuto de Ciencia de Materiales de Madrid, Spain
07/04–09/04/2011
Adsorption, cyclo-dehydrogentaion and graphene formation from molecular precursors on single-crystal surfaces.

Dr. Oleg Yazyev
University of California, Berkeley, USA
15/04–17/04/2011
One-dimensional structural irregularities in graphene - chiral edges and grain boundaries.

Dr. Gabriel Landolt
Swiss Light Source, Paur Scherrer Institut and Physik Institut, Universität Zürich, Suitzerland
17/04–19/04/2011
Spin structure investigations in topological insulators.

Dr. María José Calderón Prieto
Instituto de Ciencia de Materiales de Madrid CSIC, Spain
27/04–29/04/2011
Magnetic state and anisotropies in iron based superconductors.

Prof. Dr. Aart W. Kleijn
HIMS, University of Amsterdam, The Netherlands
02/05–05/05/2011
Dynamics of hyperthermal atoms scattered off metal surfaces.

Prof. Rogério de Sousa
University of Victoria, BC, Canada
04/05–07/05/2011
Electromagnon excitations in multiferroics.

Dr. David O'Regan
University of Cambridge, United Kingdom
07/05–10/05/2011
Nonorthogonal Wannier function optimisation: geometric aspects and linear-scaling applications to strongly-correlated materials and spectroscopy.

Dr. Valerie Anderson
Schlumberger Cambridge Research, United Kingdom
10/05–12/05/2011
Polymers under confinement.

Dr. Andrew Clarke
Schlumberger Cambridge Research, United Kingdom
10/05–12/05/2011
Polymers under confinement.

Dr. Kepa Ruiz-Mirazo
Universidad del País Vasco / Euskal Herriko Unibertsitatea, (CSIC-UPV/EHU), San Sebastián, Spain
13/05–13/05/2011
On life and its origins: when boundary conditions become more important than laws.

Dr. José Ignacio Latorre
Universitat de Barcelona, Spain
17/05–17/05/2011
Divulgación Avanzada", incluyendo la emisión del documental "Universo Extremo".

Dr. Ramón Tena-Zaera
New Materials Department, CIDETEC, Donostia-San Sebastián, Spain
27/05–27/05/2011
Nanostructured semiconductors: low cost deposition techniques and integration in solar cells.

Doctorand Danny Boettcher
Max-Planck-Institut für Mikrostrukturphysik, Germany
29/05–31/05/2011
Magnetization dynamics and equilibrium properties based on the Heisenberg model.

Prof. Bo Hellsing
Chalmers and Göteborg University, Sweden
29/05–2/06/2011
Electron-phonon interactions on metal surfaces.

Dr. Guillaume Schull
CNRS – Institut de Physique et Chimie des Matériaux de Strasbourg, France
06/06–10/06/2011
Atomic-scale control of molecular contacts.

Prof. Ricardo Garcia Garcia
Instituto de Microelectronica de Madrid, Spain
07/06–07/06/2011
Molecular resolution, nanomechanics and nanomedicine.

Dr. Laurent Bonnet
Institut des Sciences Moleculaires,
Université de Bordeaux I, France
08/06–10/06/2011
Classical reaction dynamics in quantum spirit.

Doctorand Martina Abb
University of Southampton, United Kingdom
13/06–07/07/2011
Theory of gaploading of Fanoresonances in dimer nanoantennas and dimer nanorings. Antenna and gold layer coupling with semiconductor layer in between, theoretical investigations to support experiments done in Southampton.

Dr. Carla Castellarin Cudia
Sincrotrone Elettra de Trieste, Italia
13/06–15/06/2011
A common denominator in catalysis, photovoltaic and electronic applications: the role of interfaces.

Dr. Oleg Tereshenko
Institut of Semiconductor Physics, Novosibirsk, Russia
16/06–19/06/2011
Two-dimentional plasmons and electric transport in metal layers deposited on semiconductors.

Dr. Pawel Buczek
Max-Planck-Institut für Mikrostrukturphysik, Germany
19/06–04/07/2011
Magnon electron scattering in scanning tinneling microscopy.

Dr. Eric Suarez Morell
Universidad Técnica Federico Santa María, Valparaíso, Chile
20/06–25/06/2011
Electronic structure calculations in nanotubes.

Dr. Orkhan Osmani
Universität Duisburg-Essen, Duisburg, Germany
26/06–29/06/2011
Simulation of ion tracks.

Prof. Andrey Rogach
Hong Kong University, China
09/07–14/07/2011
Morphology control and application aspects of gold nanoparticles.

Dr. Luca Perfetti
École Polytechnique, Palaiseau cedex, France
10/07–12/07/2011
Time resolved photoemission spectroscopy of bismuto.

Dr. Ziya Aliyev
Baku State University, Azerbaijan
11/07–17/07/2011
Materials physics of topological insulators.

Doctorand Soren Ulstrup
Technical University of Denmark, Denmark
11/07–19/07/2011
First principles transport calculations.

Prof. Mads Brandbyge
Technical University of Denmark, Denmark
11/07–31/07/2011
First principles transport calculations.

Prof. Antonio Hernando
Instituto de Magnetismo Aplicado ADIF, and
Universidad Complutense de Madrid, Spain
12/07–13/07/2011
Magnetism on gold-thiolate nanoparticles.

Dr. Otto Muskens
University of Southampton, United Kingdom
12/07–31/07/2011
Theory of gaploading of Fanoresonances in dimer nanoantennas and dimer nanorings. Antenna and gold layer coupling with semiconductor layer in between, theoretical investigations to support experiments done in Southampton.

Prof. Fernando Bartolomé
Instituto de Ciencia de Materiales de Aragón,
(CSIC)-Universidad de Zaragoza, Spain
13/07–13/07/2011
Magnetism of noble metal nanoparticles: a XAS and XMCD study.

Prof. Gabriel Cwilich
Yeshiva University, New York, USA
15/07–22/07/2011
Fluorescence and intensity correlations in random media.

Prof. Tomas Sikola
Brno University of Technology, Czech Republic
15/07–19/07/2011
Nanophotonics and plasmonics.

Dr. Josef Bartos
Polymer Institute of SAS, Bratislava, Slovak Republic
18/07–29/07/2011
PALS and polymer dynamics.

Doctorand Mikolaj Kajetan Schmidt
Copernico University, Torun, Poland
18/07–29/07/2011
Radiative decay of emitters in the presence of magnetic dipoles.

Dr. Aritz Leonardo
ESS Bilbao, Spain
21/07–21/07/2011
Basic principles of accelerator physics: ESS-Bilbao light ion linear accelerator.

Dr. Borja Sepulveda Martínez
Centro de Investigación en Nanociencia y Nanotecnología CIN2 CISC-ICB, Barcelona, Spain
24/07–26/07/2011
Plasmonic sensing.

Prof. Shiwu Gao
University of Gothenburg, Sweden
24/07–15/08/2011
Optical response based on time dependent density functional.

Doctorand Christine Gerstl
Institut für Festkörperforschung Jülich,
Garching, Germany
25/07–6/08/2011
Characterization of the dynamics of polyalkyleneoxides.

Dr. Caroline Genix
Université Montpellier II and CNRS Montpellier, France
25/07–30/07/2011
Effect of blending on the dynamics of a given polymer. In particular, the system poly(ethylene oxide) / poly(methyl methacrylate) has been chosen, due to the huge difference in the glass transition temperatures of the two components. A combination of quasielastic neutron scattering and fully atomistic molecular dynamics simulations is used to address the question of the dynamic miscibility in this system.

Doctorand Alexandra Fuxman
Institut für Festkörperforschung Jülich,
Garching, Germany
30/07–06/08/2011
Characterization of the dynamics of polyalkyleneoxides.

Prof. Wim Briels
University of Twente, Enschede, The Netherlands
07/08–11/08/2011
A single particle model to simulate the dynamics of entangled polymer melts.

Dr. Marco Laurati
Laboratoire Polymères et Matériaux Avancés
CNRS/Rhodia Recherche et Technologie, France
07/08–12/08/2011
Investigation, in collaboration with the company Rhodia, of the structure and dynamics of water adsorbed in polyamide (nylon) films, as a function of the percentage of crystalline phase and temperature. These studies aim at enhancing the barrier properties of polyamide with respect to the adsorption of water and other organic solvents, improving the durability of nylon-based products.

Dr. Konstantin Koch
Institute of Semiconductors Physics RAN, Novosibirsk, Russia
30/08–31/08/2011
Growth of high quality layered semiconductors.

Dr. Roberto Robles Rodríguez
CIN2: Centre d'Investigació en Nanociència i Nanotecnologia (CSIC-ICN),
Universitat Autònoma de Barcelona, Spain
07/09–8/09/2011
Electronic and magnetic properties of transition metal phthalocyanines.

Dr. Andrew Walter
Lawrence Berkeley National Laboratory, USA and
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Berlin, Germany
10/09–14/09/2011
Electronic Structure of Graphene:
Simple but Complex

Dr. Ioannis Zegkinoglou
University of Wisconsin, Madison and Lawrence Berkeley National Laboratory, USA
10/09–17/09/2011
Surface chemistry in organic solar cells.

Dr. Francisco Méndez Ruiz
Universidad Autónoma Metropolitana, Mexico
19/09–19/09/2011
Chemical reactivity and density functional theory.

Prof. Peter Saalfrank
Institut für Chemie, Universität Potsdam, Germany
18/09–20/09/2011
Elastic, inelastic, and reactive scattering of atoms and molecules from surfaces.

Prof. Julio Alonso Martín
Universidad de Valladolid, Spain
21/09–12/10/2011
Electronic structure of carbon-based materials.

Dr. Sandra García Gil
Université Paris Sud, France
26/09–29/09/2011
DFT characterization of solid surfaces and interfaces: from metallic and semiconducting to H adsorption on silicates.

Dr. José Ignacio Latorre
Universitat de Barcelona, Spain
05/10–06/10/2011
Speed of light vs speed of neutrinos

Dr. Stephen G. Hickey
Technische Universität Dresden, Institut für Physikalische Chemie und Elektrochemie, Germany
05/10–08/10/2011
Semiconductor nanoparticles: their synthesis and attachment to substrates for optoelectronic characterisation.

Dr. Laura Serkovic Loli
Université de Nancy, France
16/10–19/10/2011
Reconstruction of the (001) Al2Cu surface + Adsorption of EP-PTCDI molecules on Si(111) 7x7 and Ag(111).

Prof. Alexander Protogenov
Russian Academy of Sciences, Russia
31/10–30/11/2011
Transport properties of 3D topological insulators

Prof. Thomas Fauster
Universitat Erlangen-Nurnberg, Erlangen, Germany
04/10–06/10/2011
Image-potential states on graphene layers.

Prof. Gregor Schiwietz
Helmholtz Zentrum, Berlin, Germany
04/10–07/10/2011
Electron emission from surfaces and solids

Prof. Michel Côté
Université de Montréal, Canada
19/10–20/10/2011
Electronic properties of polymers for photovoltaic applications.

Prof. Viktor Antonov
Institute of Metal Physics,
National Academy of Sciences, Kiev, Ukraine
24/10–31/10/2011
Topological insulators.

Prof. Jeremy Baumberg
Cavendish Laboratory, University of Cambridge, United Kingdom
24/10–26/10/2011
Nanophotonics

Dr. Carlos Andrés Palma
Max-Plank-Institut für Polymerforschung,
Mainz, Germany
31/10–14/11/2011
Photodissociation of molecules in gas phase: An ab-initio study.

Doctorand Carlo Motta
Universitá di Milano-Bicocca, Italy
03/11–29/11/2011
Ab initio study of transport in nanojunctions: application to dye-sensitized solar cells.

Prof. Ivan P. Chernov
Politechnic University of Tomsk, Russia
14/11–24/11/2011
Dynamics of hydrogen in metals under external irradiation.

Prof. Peter Nordlander
Rice University, Houston, USA
17/11–22/11/2011
Fano resonances in plasmonics.

Prof. Andrei Borissov
Université Paris Sud, France
17/11–19/11/2011
Time dependent density functional theory calculations to address the optical response of plasmonic systems.

Dr. Paolo Sessi
University of Wurzburg, Germany
17/11–19/11/2011
Topological insulator.

Prof. Nicolas Lorente
Centro de Investigación en Nanociencia y Nanotecnología (CIN2-CSIC), Bellaterra, Spain
21/11–25/11/2011
Inelastic electron tunnelling spectroscopy.

Dr. Guido Fratesi
Universitá di Milano-Bicocca, Italy
21/11–24/11/2011
Strain effect on electronic and structural properties of metal nanoislands grown on reconstructed Au(111).

Doctorand Manuel Monasterio Jaqueti
Universidad Politécnica de Madrid, Spain
24/11–25/11/2011
Characterization of Nanowires.

Prof. Sydney Brenner
Howard Hughes Medical Institute,
Janelia Farm Campus, Virginia, USA
27/11–29/11/2011
Reading the Human Genome: the reconstruction of the past.

Theses

2010

Molecular dynamics of poly(ethylene-alt-propylene) melts by means of neutron scattering and simulations: Bridging the gap between fully atomistic and coarse-grained models
Roberto Perez Aparicio (UPV/EHU)
Supervisors: Juan Colmenero and Fernando Alvarez
June 2010

Doped quantum dots and MnAs wires
Carlos Echeverria-Arrondo (Universidad Pública de Navarra)
Supervisor: Andres Ayuela
June 2010

Dielectric and mechanical properties of polymers at macro and nanoscale
Clement Riedel (Université Montpellier 2 - UPV/EHU)
Supervisor: M. Philippe Tordjeman and Juan Colmenero
October 2010

2011

Structural relaxation and chain dynamics in polymer melts:
a computational investigacion on the role of the intramolecular barriers
Marco Bernabei (UPV/EHU)
Supervisor: Angel José Moreno Segurado
April, 2011

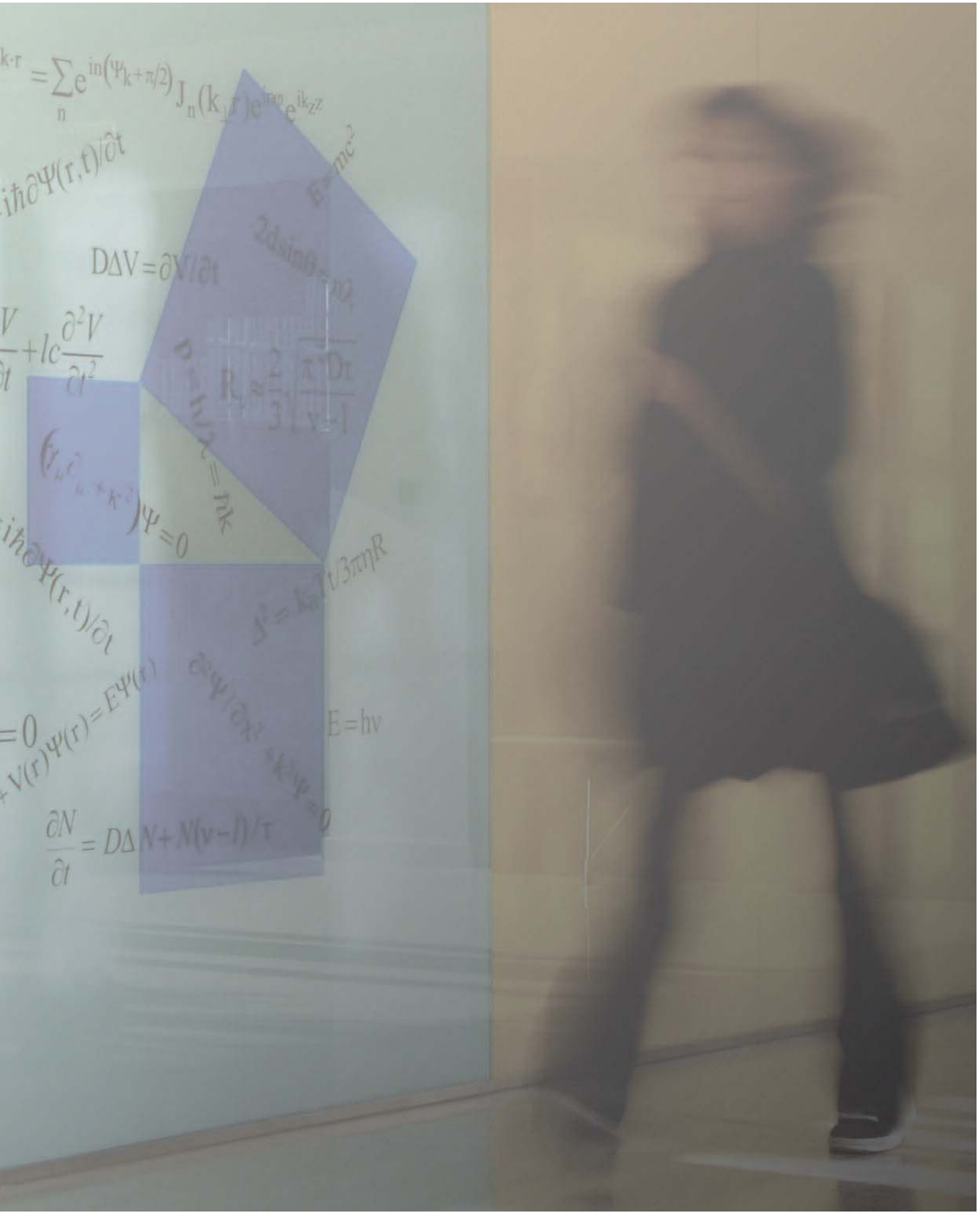
The structure and the dynamics of poly(vinyl methyl ether) PVME and PVME in concentrated water solution
Sara Capponi (UPV/EHU)
Supervisors: Arantxa Arbe and Juan Colmenero
May 2011

First principles study of the electronic and magnetic properties of defective carbon nanostructures
Elthon José Gomes Santos (UPV/EHU)
Supervisors: Daniel Sánchez Portal and Andres Ayuela Fernández
July 2011

Optical properties and high-frequency electron transport in plasmonic cavities
Olalla Pérez González (UPV/EHU)
Supervisors: Nerea Zabala and Javier Aizpurua
October 2011

Resonant Raman-Brillouin Scattering in Semiconductor and Metallic Nanostructures:
From Nano-Acoustics to Acousto-Plasmonics
Nicolas Large (UPV/EHU)
Supervisors: Javier Aizpurua and Adnen Mlayah
October 2011

Functionalized polymers as a tool for investigating the component dynamics of polymer blends
Sandra Plaza García (UPV/EHU)
Supervisor: Angel Alegría
December 2011



Seminars

2010

28/01/2010
Novel high pressure structures from first principles
Yanming Ma, State Key Lab of Superhard Materials, Jilin University, Changchun, China

29/01/2010
Cycloaddition chemistry as a tool for the preparation of valuable molecules and materials
Fernando Cossío Mora, Facultad de Química, UPV/EHU, San Sebastián, Spain

10/02/2010
Tuning molecular electroluminescence from tunnel junctions
Zhencha Dong, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, China

12/02/2010
Building integrated photovoltaics: technology and applications
Maider Machado, Fundación Inasmet, Donostia-San Sebastián, Spain

15/02/2010
Surface structural studies with MEIS.
Miguel Angel Muñoz Marques, Instituto Ciencia de Materiales de Sevilla, Spain

02/03/2010
Coexistence of ferromagnetism and superconductivity
Alexander Buzdin, Université Bourdeaux I, France

04/03/2010
Quantum Rotational Motion in mesoscopic systems
Javier Tejada Palacios, Universidad de Barcelona, Spain

25/03/2010
QM/MM studies on Cu(I) sites in zeolites and their interactions with small molecules
Pawel Rejmak, Institute of Catalysis and Surface Chemistry of Polish Academy of Science, Poland

26/03/2010
Electron cooling by diffusive normal metal - superconductor tunnel junctions
Andrey Vasenko, LPMMC, Universite Joseph Fourier and CNRS, Grenoble, France

09/04/2010
Switchable molecules on metallic surfaces
Marten Piantek, Freie Universitaet Berlin, Germany

12/04/2010
Quantum chemical study of lanthanide and actinide impurities in ionic crystals
Fernando Ruipérez Cillán, Stockholm University, AlbaNova University Centre, Stockholm, Sweden

16/04/2010
Quantum transport in nanostructures in presence of strong external perturbations:
role of high magnetic fields and electron-phonon interactions
Remi Avriller, Facultad de Ciencias, Universidad Autónoma de Madrid, Spain,
CEA Grenoble and Université Joseph Fourier, France

23/04/2010
Quantum molecular dynamics to model surface phonon polaritons nanoparticles
resonances in the THz regime
Jean Jaques Greffet, Institut d'Optique Graduate School, Institut Universitaire de France, Palaiseau, France

30/04/2010
Quantum Technologies with Circuit QED
Enrique Solano Villanueva, Facultad de Ciencia y Tecnología, UPV/EHU, Spain

07/05/2010
Self-assembly and reactivity on the graphene/Ru[0001] surface
Daniele Stradi, Universidad Autónoma de Madrid, Spain

14/05/2010
Dynamics effects in superconducting/magnetic nanostructures
José Luis Vicent López, Universidad Complutense de Madrid, Spain

17/05/2010
Electronic structure of graphene from photoemission
Aaron Bostwick, Advanced Light Source, Lawrence Berkeley National Laboratory, USA

20/05/2010
The optimized potential model for atoms and molecules
James D. Talman, University of Western Ontario, London, Canada

27/05/2010
Elastic properties of graphene and carbon nanoribbons:
a combined continuum and atomistic approach
Luciano Colombo, University of Cagliari and SLACS (INFM-CNR), Italy

08/06/2010
Phase-charge duality in Josephson junction circuits: Role of inertia and effect of microwave irradiation
Frank Hekking, Laboratoire de Physique et de Modélisation des Milieux Condensés,
Université Joseph Fourier and CNRS, Grenoble, France

09/06/2010
Rashba spin-orbit coupling at surfaces
Jürgen Henk, Max Planck Institute of Microstructure Physics, Halle, Germany

16/06/2010
Multifunctional materials design for catalysis
Avelino Corma Canós, Instituto de Tecnología Química, UPV-CSIC, Universidad Politécnica de Valencia, Spain

18/06/2010
Interaction induced edge channel equilibration
Anders Mathias Lunde, ICMM, CSIC, Madrid, Spain

22/06/2010
Surface science spectroscopy
Mario Rocca Agostino, Università degli Studi di Genova, Italy

23/06/2010
Magnetic properties of iron pnictides from spin-spiral calculations
Alexander Yaresko, Max-Planck-Institut für Festkörperforschung, Germany

25/06/2010
Novel approaches to study molecule/surface reactions
Cristina Diaz Blanco, Universidad Autónoma de Madrid, Spain

09/06/2010
Ab initio simulation of solar cells materials
Lin-Wang Wang, Lawrence Berkeley National Laboratory, California, USA

05/07/2010
Why density functional theory works and how to improve it
Kiron Burke, University of California, Irvine, USA

14/07/2010
Phonons in mixed semiconductors
Andrei Postnikov, Paul Verlaine Universite-Metz, France

19/07/2010
Electrochemical deposition of metallic films and nanoparticles on thin oxides and metallic surfaces
Mau-scheng Zei, National Central University, Taiwan

28/07/2010
Competing broken symmetries due to magnetism and unconventional superconductivity
in hybrid structures
Mario Cuoco, CNR-SPIN "E.R. Caianiello", Universita di Salerno, Italy

19/08/2010
The timely and the unexpected; spin resolved ARPES on systems with strong spin-orbit interaction
Hugo Dil, Universität Zürich, Switzerland

31/08/2010
New insights into student understanding of electric circuits and analog electronics
Stetzer MacKenzie, University of Washington, USA

06/09/2010
Photoemission study of rare gas nano-bubbles in Al(111): core-levels and plasmon excitation
Rajendra Singh Dhaka, Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

10/09/2010
Metals in graphene
Akira Ishii, Tottori University Koyama, Japan

17/09/2010
Surface defects: from mechanical properties to the origin of life
Juan Rojo, Universidad Complutense de Madrid, Spain

Seminars

2010

23/09/2010
Modern approaches to time-resolved single molecule microscopy
Steffen Ruettinger, PicoQuant GmbH, Berlin, Germany

08/10/2010
Novel phenomena at high pressure
Artem R. Oganov, Stony Brook University, New York, USA

18/10/2010
Strongly emitting colloidal nanocrystals and their assemblies
Nikolai Gaponik, Technical University Dresden, Germany

21/10/2010
Euler buckling instability and enhanced current blockade in suspended single-electron transistors
Fabio Pistolesi, Université Bordeaux/CNRS, Talence, France

22/10/2010
Water-solid interfaces at ambient conditions
Jordi Fraxedas Calduch, Centre d' Investigació en Nanociència i Nanotecnologia CIN2(CSIC-ICN), Barcelona, Spain

29/10/2010
At the nexus of physics and physiology
Peter Apell, Chalmers University of Technology, Goteborg, Sweden

03/11/2010
Magnetism in funcionalised nanoparticles
Antonio Hernando Grande, Instituto de Magnetismo Aplicado, UCM-CSIC-ADIF, Madrid, Spain

18/11/2010
Plasmonics: integrated devices and cavities for biosensing applications
Pol Van Dorpe, IMEC, Leuven, Belgium

19/11/2010
Collective phenomena in semiconductor microcavities
Ivan Shelykh, University of Iceland, Iceland

02/12/2010
Cellular automata and GPU computations
Néstor Ferrando Jódar, Universidad Politécnica de Valencia, Spain

09/12/2010
Self-assembly and electronic properties of macromolecular systems:
ordered ultrathin porphyrin layers vs hierarchically assembled eumelanin thin films
Patrizia Borghetti, Università Cattolica del Sacro Cuore, Brescia, Italy

2011

14/01/2011
Quantum escape processes for driven systems
Alvise Verso, Ulm University, Germany

25/01/2011
Attosecond electron dynamics in solids
Ralph Ernstorfer, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

04/02/2011
Dynamics of DNA and DNA-Hydration water on the picosecond time-scale
Guido Goracci, University of Perugia, Italy

18/02/2011
Orbital magnetoelectric effect in insulators
Ivo Souza, University of California, Berkeley, USA

24/02/2011
Helium spin echo spectroscopy as a technique for surface dynamical studies: results and interpretation
John Ellis, Cavendish Laboratory, University of Cambridge, United Kingdom

24/02/2011
Influence of macromolecular crowding on protein stability
Clémence Le Coeur, Laboratoire de Physique des Solides, Paris, France

03/03/2011
Using synchrotron radiation to shed light on solar cells
Franz J. Himpsel, University of Wisconsin Madison, United Status

04/03/2011
Ultrafast charge transfer at graphene surfaces
Dietrich Menzel, Technische Universität München and Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

11/03/2011
Nearfield optical plasmonics: from single and coupled particles to extended metamaterials
Ralph Vogelgesang, Max-Planck-Institut für Festkörperforschung, Germany

18/03/2011
Structural and chemical effects of charge-transfer across metal-organic interfaces
Roberto Otero Martín, Universidad de Autónoma de Madrid, Spain

23/03/2011
Optics of Graphene
Alexey Kuzmenko, Université de Genève, Switzerland

23/03/2011
The methodology of research in physics education used in the university of Udine
Marisa Michelini, University of Udine, Italy

31/03/2011
Nanocrystals: past, present and future
Alexander Eychmüller, Technical University of Dresden, Germany

01/04/2011
Fast ion diffraction on crystal surfaces
Maria Silvia Gravielle, Instituto de Astronomía y Física del Espacio, Universidad de Buenos Aires, Argentina

05/04/2011
New approach to studying the interaction between charged particles and its impact on science
Elena Bichoutskaia, School of Chemistry, University of Nottingham, United Kingdom

08/04/2011
Adsorption, cyclo-dehydrogentaion and graphene formation from molecular precursors on single-crystal surfaces
José Angel Martín Gago, Insitituto de Ciencia de Materiales de Madrid, Spain

15/04/2011
Electron transport through carbon nanostructures
Martti Puska, Aalto University School of Science and Technology, Finland

15/04/2011
One-dimensional structural irregularities in graphene – chiral edges and grain boundaries
Oleg Yazyev, University of California, Berkeley, USA

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Magnetic state and anisotropies in iron based superconductors
María José Calderón Prieto, Instituto de Ciencia de Materiales de Madrid CSIC, Spain

04/05/2011
Radical interactions at surfaces
Aart W. Kleijn, HIMS, University of Amsterdam, The Netherlands

05/5/2011
Electromagnon excitations in multiferroics
Rogério de Sousa, University of Victoria, B.C., Canada

09/05/2011
Nonorthogonal Wannier function optimisation: geometric aspects and linear-scaling applications to strongly-correlated materials and spectroscopy
David O'Regan, University of Cambridge, United Kingdom

13/05/2011
On life and its origins: when boundary conditions become more important than laws
Kepa Ruiz-Mirazo, UPV/EHU (CSIC-UPV/EHU), Donostia-San Sebastián, Spain

17/05/2011
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José Ignacio Latorre, Universitat de Barcelona, Spain

27/05/2011
Nanostructured semiconductors: low cost deposition techniques and integration in solar cells
Ramón Tena-Zaera, New Materials Department, CIDETEC, Donostai-San Sebastián, Spain

08/06/2011
Atomic-scale control of molecular contacts
Guillaume Schull, CNRS – Institut de Physique et Chimie des Matériaux de Strasbourg, France

14/06/2011
A common denominator in catalysis, photovoltaic and electronic applications: the role of interfaces
Carla Castellarin Cudia, Sincrotrone Elettra de Trieste, Italy

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Morphology control and application aspects of gold nanoparticles
Andrey Rogach, Hong Kong University, China

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Dynamics of electronic states at the surface of bismuth
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Magnetism of noble metal nanoparticles: a XAS and XMCD study
Fernando Bartolomé, Instituto de Ciencia de Materiales de Aragón, (CSIC)-Universidad de Zaragoza, Spain

21/07/2011
Basic principles of accelerator physics: ESS-Bilbao light ion linear accelerator
Aritz Leonardo, ESS Bilbao, Spain

26/07/2011
Strategies to improve the limit of detection in nanoplasmonic label free biosensing
Borja Sepulveda Martínez, Centro de Investigación en Nanociencia y Nanotecnología CIN2 CISC-ICB, Barcelona, Spain

01/08/2011
New challenges and opportunities in nanoplasmonics: from transformation optics cavity design to applications in biosensing and solar light harvesting
Stefan Maier, Imperial College London, United Kingdom

2011

04/08/2011
Quantum and semiclassical description of surface plasmons: electronic damping and screening
Shiwu Gao, University of Gothenburg, Sweden

08/09/2011
Electronic and magnetic properties of transition metal phthalocyanines
Roberto Robles Rodríguez, CIN2: Centre d'Investigació en Nanociència i Nanotecnologia (CSIC-ICN)
Universitat Autònoma de Barcelona, Spain

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Electronic Structure of Graphene: Simple but Complex
Andrew Walter, Lawrence Berkeley National Laboratory, United States and
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

19/09/2011
Chemical Reactivity and Density Functional Theory
Francisco Méndez Ruiz, Universidad Autónoma Metropolitana, Mexico

20/09/2011
Adsorbate quantum dynamics at surfaces treated by system-bath methods
Peter Saalfrank, Institut für Chemie, Universität Potsdam, Germany

29/09/2011
DFT characterization of solid surfaces and interfaces: from metallic and semiconducting
to H adsorption on silicates
Sandra García Gil, Université Paris Sud, France

03/10/2011
Interaction and interference in molecular electronics: a density matrix approach
Andrea Donarini, Institute of Theoretical Physics, University of Regensburg, Germany

05/10/2011
Auger angular distribution effects induced by heavy ions
Gregor Schiwietz, Helmholtz Zentrum, Berlin, Germany

05/10/2011
Image-potential states on graphene layers
Thomas Fauster, Universitat Erlangen-Nurnberg, Erlangen, Germany

05/10/2011
Speed of light vs speed of neutrinos
José Ignacio Latorre, Universitat de Barcelona, Spain

06/10/2011
Semiconductor nanoparticles: their synthesis and attachment to substrates for optoelectronic
characterisation
Stephen G. Hickey, Technische Universität Dresden, Institut für Physikalische Chemie und Elektrochemie, Germany

17/10/2011
Reconstruction of the (001) Al2Cu surface + Adsorption of EP-PTCDI molecules on
Si(111) 7x7 and Ag(111)
Laura Serkovic Loli, Université de Nancy, France

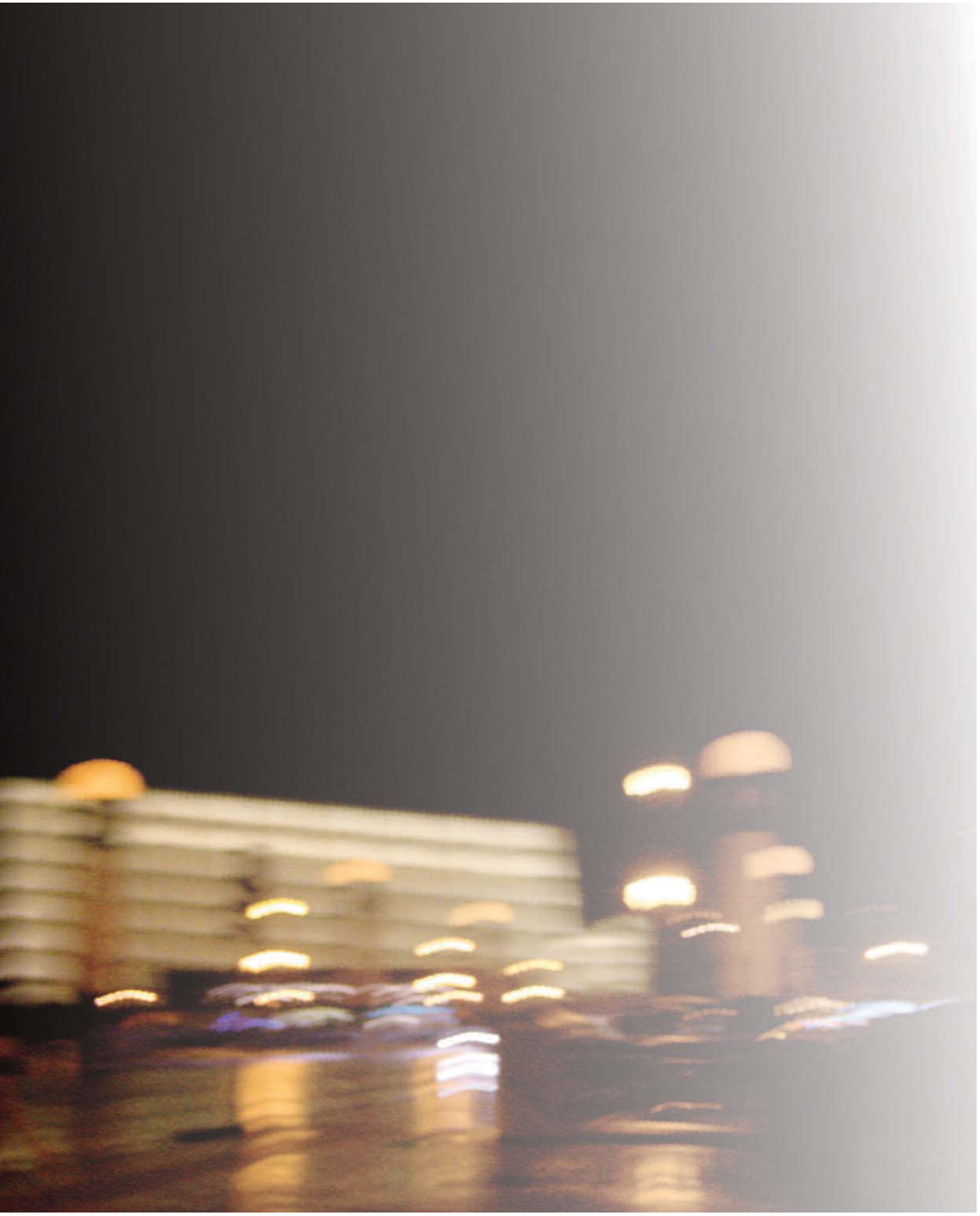
20/10/2011
Electronic properties of polymers for photovoltaic applications
Michel Côté, Université de Montréal, Canada

21/11/2011
Fano resonances and quantum effects in plasmonics
Peter Nordlander, Rice University, Texas, USA

22/11/2011
Strain effect on electronic and structural properties of metal nanoislands
grown on reconstructed Au(111)
Guido Fratesi, Universitá di Milano-Bicocca, Italy

28/11/2011
Reading the Human Genome: the reconstruction ot the Past
Sydney Brenner, Janelia Farm Campus, Howard Hughes Medical Institute USA

15/12/2011
Optics, self assembly, and evolution of nanostructural colors in birds and insects
Richard O. Prum, Yale University, Peabody Museum of Natural History, Connecticut, USA



Workshops

2010

2011

SOFTCOMP – DYNACOP Workshop

New Trends in Polymer Rheology: Complex Architectures and Complex Environments

Abril 12-14, 2010

ORGANIZERS

Prof. J. Colmenero (DIPC, Donostia-San Sebastián, Spain)
D. Richter (Forschungszentrums Jülich, Germany)

Polymer materials are evolving from more or less simple liner polymer systems towards multi-component and nano-structured systems, involving in many cases polymers with complex architectures as well. The idea of the workshop is to discuss the impact of this complexity on the rheological concepts and theories. New theoretical approaches and simulations will be revised at the light of recent experimental results from both macroscopic and microscopic (molecular) experimental techniques.

In connection with the European Network of Excellence, SoftComp and with the Marie Curie Action, DYNACOP, this workshop is now being organized by Professor Juan Colmenero and by Professor Dieter Richter – general coordinator of SoftComp. The workshop will take place in the Donostia International Physics Center (DIPC), San Sebastián, Spain. In the spirit of this type of workshops the number of participants will be limited to about 60 and there will be only invited lectures (see below) and oral contributions (of the order of 20).

CONTRIBUTIONS

Christian Bailly (Université catholique de Louvain, Belgium)
François Tournilhac (Ecole Supérieur de Physique et Chimie, Paris, France)
Dimitris Vlassopoulos (FORTH-Hellas, Heraklion, Greece)
Giuseppe Marrucci (Universita' degli Studi di Napoli, Italy)
Nikos Hadjichristidis (University of Athens, Greece)
Tom McLeish (Durham University, UK)
Jean-Louis Barrat (Universite Claude Bernard Lyon 1, France)
Angel Moreno (Materials Physics Center, UPV/EHU-CSIC, San Sebastián, Spain)
John M. Torkelson (Northwestern University, Illinois, USA)
Gerald Schneider (Forschungszentrums Jülich, Germany)
Francois Boue (LLB, CEA-CNRS Saclay, France)
Wolfgang Paul (Martin-Luther-Universität, Halle, Germany)
Gustavo Schwartz (Materials Physics Center, UPV/EHU-CSIC, San Sebastián, Spain)
Dieter Richter (Forschungszentrums Jülich, Germany)
Juan Colmenero (Materials Physics Center, UPV/EHU-CSIC and DIPC, San Sebastián, Spain)
Angel Alegría, "Dielectric Spectroscopy" (Materials Physics Center, UPV/EHU-CSIC, San Sebastián, Spain)
Reiner Zorn, "Neutron Scattering" (Forschungszentrums Jülich, Germany)

Summer School on Computational Materials Sciences

June 28 - July 3, 2010

ORGANIZERS

I. Abrikosov (Linköping University, Sweden)
J. Neugebauer (Maz Planck Institut für Eisenforschung, Germany)
A. Ayuela (DIPC and Unidad de Física de los Materiales, Centro Mixto CSIC-UPV/EHU, Spain)
P. Cabrera-Sanfelix (DIPC, Donostia-San Sebastián, Spain)

The Summer School on Computational Materials Sciences aims at the identification and promotion of the common elements developed in theoretical and computational studies of materials properties across materials types, metals, ceramics, materials for new energy technologies, electronic materials and minerals. To accomplish this goal, the School brings together leading experts from a wide spectrum of materials simulations including theory, modeling, and computation, engaged in the study of a broad range of materials properties.

Therefore, this School provides a forum for exposing young researchers and students to most recent state-of-the-art theoretical and computational developments in studying, understanding, and predicting the properties of materials. Also, the School encourages interdisciplinary contributions, such as between the fields of condensed matter physics and applied materials sciences, chemistry, metallurgy, etc.

The emphasis of the School on Computational Materials Sciences will be on attracting scientists, students, and young researchers in the fields of basic science, e.g., electronic structure and related properties, assessing alloy phase diagrams, semiconductor physics, mineral science, and phenomenology. The emphasis on cross-fertilization of subject matter and the interdisciplinary character of the presentations make this meeting unique.

CONTRIBUTIONS

D. Alfe (University College London, United Kingdom)
J. A. Alonso (Universidad de Valladolid, Valladolid, Spain)
M. Asta (University of California, Davis, USA)
K. Burke (University of California, Irvine, USA)
R. Diez-Muiño (DIPC, CFM-UPV/EHU, Donostia-San Sebastián, Spain)
R. Drautz (ICAMS, Bochum, Germany)
S. L. Dudarev (UKAEA Euratom Fus Assoc, United Kingdom)
C. Freysoldt (Max-Planck-Institut, Düsseldorf, Germany)
A. George (Ecole Polytechnique, Paris, France)
A. Hartmeier (ICAMS, Bochum, Germany)
T. Hickel (Max-Planck-Institut, Düsseldorf, Germany)
P. Korzhavyi (Royal Institute of Technology (KTH), Sweden)
P. Ordejón (Centre d'Investigació en Nanociéncia i Nanotecnología (CIN2), Barcelona, Spain)
V. Ozolins (University of California, Los Angeles, USA)
J. von Pezold (Max-Planck-Institut, Düsseldorf, Germany)
P. Rinke (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)
A. Ruban (Royal Institute of Technology (KTH), Sweden)
D. Sanchez-Portal (DIPC, CFM-UPV/EHU, Donostia-San Sebastián, Spain)
S. I. Simak (Linköping University, Sweden)
C. van de Walle (University of California, Santa Barbara, USA)

Fourth International Workshop Photonic and Electronic Materials

July 5-7, 2010

ORGANIZERS
Rolindes Balda (UPV/EHU-CSIC, DIPC, Spain)
Joaquín Fernández (UPV/EHU-CSIC, DIPC, Spain)
Paras N. Prasad (Institute for Lasers and Biophotonics, University at Buffalo, The State University of New York, USA)

INTERNATIONAL ADVISORY COMMITTEE
Georges Boulon (Claude Bernard Lyon I University, France)
Peter Günter (ETH-Zürich, Switzerland)
Sajeev John (University of Toronto, Canada)
David Levy (ICMM, CSIC, Spain)
Manuel Nieto-Vesperinas (ICMM, CSIC, Spain)
Ken-ichi Ueda (Institute for Laser Science, University of Electro-Communications, Japan)
Martin Wegener (Karlsruhe Institute of Technology, Germany)

In the last years a wide variety of research activities linked with the interaction between light and matter have developed important applications in fields such as telecommunications, information technology, medical diagnostics and treatment, environment control etc. Among all the applications for the foreseeable future, those based on the non linear optical properties of matter are specially promising. Moreover, science and technology breakthroughs in the 21st Century are more likely to occur at the interface of disciplines. Recently much interest has been focused on Biophotonics defined as the interface of photonics and biological sciences. It is a new frontier, offering tremendous prospects for optical diagnostics as well as light activated therapy, surgery, biosensing, and restoration of biological functions. The demand for suitable materials (optical storage systems, systems with artificial non linearities, multipolar structures, new waveguides, photonic bandgaps, rare earth activated nano crystals, activated fibers...) and new techniques for detection in these fields are continuously growing.

The purpose of this workshop was to gather researchers from crossed fields and horizons (universities, laboratories and industries), to provide a much needed forum for the critical assessment and evaluation of recent developments in photonic materials (inorganic, organic, polymeric, biological, ..) and molecular devices. It also gaveparticipants an insight on future advances and research possibilities in these fields and an opportunity for starting fruitful collaborations.

CONTRIBUTIONS

Chairperson S. John

Nonlinear Optics, Nanophotonics and Biophotonics:
New Interfaces to Meet 21st Century Technical Challenges
P.N. Prasad (Institute for Lasers, Photonics and Biophotonics, University at Buffalo, The State University of New York, USA)

Near field Photonic Forces on Dielectric and Magnetodielectric Small Particles
M. Nieto-Vesperinas (Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC Madrid, Spain)

Optical microresonators for optoelectronic and biomedical applications
G. Righini (Istituto di Fisica Applicata Nello Carrara (IFAC CNR), Firenze, Italy)

Chairperson I. Ledoux

Organic electro-optical microring resonators for highly integrated optics
P. Günter (Institute of Quantum Electronics, Swiss Federal Institute of Technology, Zürich, Switzerland)

The Benefits of Single Domain Ferroelectric Nanoparticles in Disparate Optical Devices
D. R. Evans (Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio, USA)

Terahertz waves for materials testing and security
C. Medrano (Rainbow Photonics AG, Zurich)

Chairperson P. Günter

Multifunctional molecular materials and nanostructures for photonics: from molecular engineering to optoelectronic devices
I. Ledoux (Institut d´Alembert Ecole Normale Supérieure de Cachan, France)

Artificially designed materials using metal nano-objects
C. N. Afonso (Laser Processing Group, Instituto de Optica, CSIC, Madrid, Spain)

Chairperson M. Wegener

Optical Cavity Control of the Exciton Diffusion in Organic Photovoltaic cells
J. Martorell (ICFO-Institut de Ciencies Fotoniques, Castelldefels, Spain and Universitat Politècnica de Catalunya, Terrassa, Spain)

Spatio-temporal properties of femtosecond laser-induced plasmas:
Control of laser structuring of dielectrics via non-linear absorption
J. Solís (Instituto de Óptica, CSIC, E-28006 Madrid, Spain)

Chairperson P.N. Prasad

Photonic Band Gap Materials: Light Control at Will
S. John (Department of Physics, University of Toronto, Canada)

3D Photonic Metamaterials and Transformation Optics
M. Wegener (DFG-Center for Functional Nanostructures and Karlsruhe School of Optics & Photonics, Karlsruhe Institute of Technology, Karlsruhe, Germany)

Plasmonic antennas as building blocks for compact optical switchers
J. Aizpurua (Centro de Física de Materiales, CSIC-UPV/EHU, Donostia-San Sebastián, Spain)

Chairperson C.N. Afonso

Tuning the Lasing in Self-assembled Photonic Structures
C. López (Instituto de Ciencia de Materiales de Madrid , CSIC, Madrid, Spain)

Eutectics as self-organized systems for metamaterials and photonic applications
R.I. Merino (Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza-CSIC, Zaragoza)

Nonlinearities in metamaterials from self assembled and holographically defined templates
A. M. Urbas (Air Force Research Laboratory, Wright Patterson Air Force Base, Ohio, USA)

Chairperson G. Righini

Research of circadian response for white lighting with Ce3+-doped glass phosphor and UV/blue LEDs
G. Boulon (Laboratoire de Physico-Chimie des Matériaux Luminescents, Université de Lyon, France)

Optical Fibers and Glass-Ceramics for infrared photonics
J. L. Adam (Equipe Verres et Céramiques, Université de Rennes, France)

Chairperson J.L. Adam

Glass-ceramic planar waveguides
A. Chiasera (Istituto Fotonica e Nanotecnologie, Gruppo CSMFO, Università degli studi di Trento, Italy)

Molecular configuration transitions of a nematic liquid crystal encapsulated in hybrid silicas
D. Levy (Instituto de Ciencia de Materiales de Madrid - ICMM, CSIC, Spain)

Chairperson D. Levy

Giant Micro-Photonics : Domain Controlled Optical Materials
T. Taira (Institute for Molecular Science, Okazaki, Japan)

Superfluidity in out-of-equilibrium condensates: microcavit polaritons
L. Viña (Dept. Física de Materiales, Universidad Autónoma de Madrid, Spain)

Chairperson G. Boulon

Integrated amplifiers and lasers in Al2O3:Er3+ thin films on a silicon chip
M. Pollnau (Integrated Optical MicroSystems Group, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands)

One and two photon pumped random lasing in dye doped silica-based inhomogeneous systems
S. García-Revilla (ETS Ingeniería de Bilbao, UPV/EHU, Bilbao, Spain)

Excited state dynamics of metal –polybipiridine complexes investigated by ultrafast optical spectroscopies
Andrea Cannizzo (Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Fédérale de Lausanne, Switzerland)

International Soft Matter Conference 2010

July 5-8, 2010, Granada, Spain

ORGANIZING COMMITTEE
Chairperson Roque Hidalgo Alvarez

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Alberto Martin Molina
Antonio Martin Rodriguez
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Juan de Vicente Alvarez de Manzaneda
Victor Mosquera Tallon
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Marie Pierre Krafft (France)
Shlomo Magdassi (Israel)
Magdaleno Medina-Noyola (Mexico)
Fernando Oliveira (Brasil)
Dieter Richter (Germany)
Jan Vermant (Belgium)
Dimitri Vlassopoulos (Greece)
Darsh Wasan (USA)
Erik Wassne

This conference brought together students and scientists interested in soft matter systems such as polymers, colloids, surfactants, membranes, biomaterials and their composites. Soft Matter is characterized by multi component mixtures, large ranges of length and time scales and many interacting degrees of freedom, leading to complex structures, phase behaviour and dynamics. This implies high sensitivity to external fields and ubiquitous and significant non-equilibrium phenomena.

Soft matter science requires an interdisciplinary approach connecting theoretical, computational and experimental physics, physical chemistry, material science and biology. A special focus of discussion in this context will be the application of soft matter concepts to biological and biomimetic systems.

In this field, basic science and a broad range of modern technological application encompassing also many aspects of nano-science are closely related. These links will be emphasized during this conference, thereby fostering the exchange between academia and industry.

There were four types of presentations: plenary talks, invited and contributed talks, and posters. These will be chosen by the program committee in cooperation with the advisory board. The contributed talks will be selected from submitted abstracts.

cont'd

CONTRIBUTIONS

2010

Biophysics

G. Büldt (Forschungszentrum Jülich, Germany)
Protein Dynamics and Intermediate States in the Working Cycles of Retinal Proteins

P. Fratzl (Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Germany)
The plant cell wall as a natural polymeric material: structure, mechanical properties, actuation

P.A. Janmey (Vagelos Research Laboratories, Philadelphia, USA)
Non-linear rheology of biopolymer networks

K. Kinosita, Jr. (Waseda University, Tokyo, Japan)
Rotating Protein Machines

P. Nassoy (Institut Curie, Paris, France)
Homeostasis and Rheology of the cellular membrane

Colloids

S. Fraden (Brandeis University, Waltham, USA)
The PhaseChip: Separating Nucleation and Growth with Microfluidics

C. Bechinger (Universität Stuttgart, Germany)
Colloidal monolayers on quasiperiodic light fields

E.R. Weeks (Math & Science Center, Atlanta, USA)
The colloidal glass transition in confinement

M. Dijkstra (Utrecht University, The Netherlands)
Directing colloidal self-assembly by templates, electric fields, and depletion attractions

P. Bartlett (University of Bristol, United Kingdom)
The puzzle of sudden gel collapse – what is going on?

Dynamics of Complex Fluids

P.D. Olmsted (University of Leeds, United Kingdom)
The effects of boundaries and interfaces on shear banding in complex fluids

W. Briels (University of Twente, The Netherlands)
Coarse grain simulations of rheological properties of polymer liquids; from blobs to single particle models

M. Cloitre (Ecole Supérieure de Physique et Chemie Industrielles, Paris, France)
Micromechanics of soft glasses

H. Seto (Institute of Materials Structure Science, Japan)
Multilamellar structures induced by antagonistic salt added to a binary mixture of water and organic solvent

T. Squieres (University of California, USA)
Microrheology of phospholipid monolayers: direct visualization of stretching, flowing, yielding and healing

Membranes

T. Auth (Forschungszentrum Jülich, Germany)
Biomembranes: membrane proteins and active cytoskeleton

F. Brochard-Wyart (Institut Curie, Paris, France)
Mechanics of Cellular Aggregates

J. Rädler (Ludwig-Maximilians-Universität, München, Germany)
Soft matter nanosystems for gene and drug delivery

C.R. Safinya (University of California, USA)
Tau Protein Directed Assembly in Neuronal Systems

2010

Polymers

M. Rubinstein (University of North Carolina, USA)
Polymer Physics of Airway Surface Layer in Lungs

F. Graeter (Shanghai Institutes for Biological Sciences, China)
Force distribution through complex molecules: clues to biomechanics and function

A. Moreno (Centro de Física de Materiales, San Sebastián, Spain)
Computer simulations of block copolymer dynamics: Soft confinement in nanostructured mesophases

E. van Ruymbeke (Université Catholique de Louvain, Belgium)
Telechelic Linear and Star Polymer Melts: Linear Rheology and Modelling

R. Biehl (Forschungszentrum Jülich, Germany)
Is dynamics important for protein function?

Self-Assembly

I.W. Hamley (The University of Reading, United Kingdom)
Amyloid Peptides and Peptide Copolymers: From self-assembly, towards therapeutics

C. Ligoure (University of Montpellier, France)
Morphology driven failure mode transition in self-assembled transient networks

M. Miguel (University of Coimbra, Portugal)
Mixtures of DNA with cationic surfactants and proteins: gels and gel nanoparticles

D. Andelman (Tel Aviv University, Israel)
Block copolymers at surfaces: patterns, templates and applications

E. Zaccarelli (Universita di Roma "La Sapienza", Italy)
Laponite as a complex colloid: aggregation, gel and glass formation

Surfaces and Interfaces

G. Fragneto (Institut Laue-Langevin (ILL), France)
Bio-films by neutron scattering: a perspective

L. Léger (CNRS & Université Paris-Sud, France)
Grafted polymer layers: a way to control adhesion and friction

M. Quesada-Perez (University of Jaén, Spain)
The effect of ion size on colloidal forces: A Monte Carlo simulation study

P.S. Clegg (University of Edinburgh, United Kingdom)
How robust are particle-stabilized emulsions and bijels?

S. Dietrich (Max-Planck-Institut für Metallforshung, Stuttgart, Germany)
The critical Casimir effect: measuring and tuning femto-Newton forces

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Soft Nanotechnology

S. Herminghaus (Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany)
Collective behaviour and self-organization in fluid micro-systems

J. Bibette (ESPCI, Paris, France)
Microorganism Growth Kinetic Variability in Droplets

S.K. Kumar (Columbia University, New York, USA)
Nanoparticle Amphiphiles

S. Lemay (Kavli Insitute of Nanoscience, Delft, The Netherlands)
Electrochemical nanofluidics: Mesoscopic and single-molecule limits

J. Veciana (Instituto de Ciencia de Materiales de Barcelona (CSIC), Spain)
Soft organic thin films, based on nanostructured polymeric composites, as ultra sensitive piezoresistive materials and their applications

Catedra Collège de France - Fundación Marcelino Botín

Nanoscience:
Chemistry and Physics Behind Supramolecular Science

July 16, 2010

ORGANIZER
Prof. Felix Yndurain (Universidad Autónoma de Madrid, Spain)

LOCAL ORGANIZERS
Dr. Daniel Sánchez-Portal (DIPC, Centro de Física de Materiales CSIC, UPV/EHU, Spain)
Prof. Fernando Cossio (UPV/EHU, Spain)

CONTRIBUTIONS

Iñigo Saenz de Miera (Fundación Marcelino Botín, Santander, Spain)
Pedro Miguel Etxenike (DIPC, Donostia-San Sebastián, Spain)

Jean Mari Lehn (Collège de France, Paris, France)
Nanoscience and Nanotechnology- The Self Organisation Approach
Chairman: Pedro Miguel Etxenike

Alexander Bittner (CIC NanoGUNE Consolider, Donostia-San Sebastián, Spain)
Self-and "not so self"-assemby: Plant virus Hybrids and peptides
Chairman: Txema Pitarke

Igor Nabiev (CIC NanoGUNE Consolider, Donostia-San Sebastián, Spain)
Chemistry and Physics behind Energy Transfer from Nanostructures to Bio-Supramolecular Photosensitive Complexes
Chairman: Andrés Arnau

Tomás Torres (Universidad Autónoma de Madrid, Spain)
Phthalocyanines: old dyes, new materials. Putting color in nanotechnology
Chairman: Fernando Cossio

Rubén Pérez (Universidad Autónoma de Madrid, Spain)
Understanding surface chemistry with STM and AFM: from single-atom chemical identification to heterofullerene. Synthesis with planar aromatic precursors
Chairman: Enrique Ortega

Carmen Ocal (Instituto de Ciencias de Materiales de Barcelona, CSIC, Spain)
Functionalization by self-assembling: a route for selective growth and tuned surface properties
Chairman: Daniel Sanchez Portal

Miquel Salmerón (Lawrence Berkeley National Laboratory, California, USA)
Fundamental studies of molecular electronics: ultra-flat transistors with semiconducting self-assembled monolayers of oligothiophenes
Chairman: Felix Yndurain

Workshop on Inelastic Transport Phenomena

September 1-3, 2010

ORGANIZERS
Thomas Frederiksen (DIPC, Spain)
Aran Garcia-Lekue (DIPC, Spain)

STEERING COMMITTEE
Prof. Andres Arnau (DIPC, Centro de Física de Materiales (CSIC-UPV/EHU), Spain)
Dr. Nicolas Lorente (CIN2: Centre d'Investigació en Nanociència i Nanotecnologia (CSIC-ICN), Spain)
Prof. Stephan Roche (CEA, SP2M, France)
Dr. Daniel Sanchez-Portal (DIPC, Centro de Física de Materiales (CSIC-UPV/EHU), Spain)

2010

The Workshop on Inelastic Transport Phenomena aims at the identification and promotion of the common elements developed in experimental and theoretical studies of inelastic transport phenomena, which are fundamental for the development of nanoelectronics. To accomplish this goal, the workshop brought together leading experts from the field of inelastic transport, including theoriticians and experimentalists with outstanding achievements within the theme of the workshop.

This workshop provided a forum for experts to expose the most recent state-of-the-art theoretical and experimental developments in studying, understanding, and predicting the inelastic properties of electronic transport. Discussion between experts was strongly encouraged, with special emphasis on the cross-fertilization between different subfields of inelastic transport. This workshop also aimed to attract students and young researchers in the field.

The call for participation will be mainly directed to students, young researches and scientists specialized on inelastic transport phenomena. The number of participants was limited to 40, in order to ensure a maximum interaction between all the scientists participating. Attendance of graduate students and postdocs was strongly encouraged through the inclusion of a poster session.

Scientific Objectives
The objective of this event was to gather experts in the field of electronic transport at the nanoscale, with special emphasis on the investigation of inelastic processes. In particular, great emphasis will be placed on the study and theoretical investigation of energy transfer processes between moving electrons and atomic nuclei, i.e., vibrational excitations and Joule effect in nanojunctions. Other inelasic effects such as those related to electron-electron interaction or spinflip processes wil also be discussed. The most relevant experimental aspects of the field will be covered by experts on scanning tunneling microscopy and break-junction technique.

Since the seminal work of I. K. Yanson, inelastic spectroscopy has become a standar experimental technique which allows to determine accurately the vibrational density of states of the materials forming a nanojunction. Equally, this technique allows the measurement of electron-phonon coupling as a function of incident electron energy. In recent years, this technique has been used to characterize molecular junctions and nanocontacts. In such systems, the excitation of vibrations localized in the contact region and the consequent detection of changes in the resistance of the junction, allow to determine the type of molecule in the junction, the geometry of its bond to the contacts and the nature of the chemical bonds involved in electronic propagation. For all these reasons, inelastic spectroscopy is believed to be an important technique in the emerging field of nanoelectrons.

CONTRIBUTIONS

Prof. Nicolas Agraït (Universidad Autónoma de Madrid (UAM), Spain)
Inelastic Electron Tunneling Spectroscopy and Transport in Single molecules

Dr. Maite Alducin (Centro de Física de Materiales CFM-MPC, San Sebastian, Spain)
The vibrational inelastic electron tunneling spectroscopy of O_2 on Ag(110): what can we learn on the electronic structure

Dr. Mads Brandbyge (Technical University of Denmark, Denmark)
Current-driven runaway-instabilities in molecular bridges

Dr. Jorge Cerdá (ICMM, Madrid)
IETS simulations under tunneling regime: molecules adsorbed at surfaces and STM tips

Dr. Luis Foà Torres (FaMAF, Universidad Nacional de Córdoba, Argentina)
AC transport in carbon-based devices: unveiling novel phenomena in a world made of carbon

Prof. Jean-Pierre Gauyacq (LCAM, CNRS-Paris Sud, France)
Magnetic transitions induced by tunnelling electrons in individual adsorbates

Dr. Rafael Gutierrez (Dresden University of Technology, Germany)
Charge transport in dynamical environments: applications to DNA and organic stacks

Prof. Wilson Ho (University of California Irvine, USA)
Atomic Scale Inelastic Tunneling Phenomena

Dr. Hiroyuki Ishii (University of Tsukuba, Japan)
Inelastic transport through phonon-vibrating carbon nanotubes-Scattering times and temperature-dependent decoherence effects

Prof. Abraham Nitzan (Tel Aviv University, Israel)
Inelastic transport, heating and cooling in molecular junctions

Dr. Frederico Novaes (Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain)
Simulations of inelastic conductance in magnetic adsorbates from first principles

Dr. Frank Ortmann (CEA, Grenoble)
Charge Transport in Organic Crystals

Prof. Jose-Ignacio Pascual (Freie Universität Berlin, Germany)
Electron transfer phenomena in quantum transport through molecules on surfaces

Dr. Magnus Paulsson (Kalmar University, Sweden)
First-principles description of inelastic transport in atomic and molecular wires

Dr. Alessandro Pecchia (University of Rome, Italy)
Heating and cooling effects in molecular electronics

Prof. Mats Persson (University of Liverpool, UK)
Inelastic spin excitations in tunneling from electronic structure calculations

Prof. Jan van Ruitenbeek (Leiden University, The Netherlands)
Experimental model systems: inelastic scattering and shot noise

Dr. Daniel Sanchez-Portal (DIPC and CFM-MPC, San Sebastian, Spain)
Functionalized STM tips: propensity rules and its influence on the IETS of single-molecules

Dr. Carlos Untiedt (Universitat d'Alacant, Spain)
Transport through atomic-contacts, e-ph and e-e interactions

Dr. Lucia Vitali (DIPC, San Sebastian, Spain)
Local effects on Inelastic Electron Tunneling Spectroscopy at single molecular junctions

2010

Dynamical Processes in Irradiated Materials

July 26-28, 2010

ORGANIZERS
Prof. Andres Arnau (DIPC, Centro de Física de Materiales CSIC, UPV/EHU, Spain)
Prof. Emilio Artacho (Earth Sciences Department, University of Cambridge, UK)
Dr. Iñaki Juaristi (DIPC, Centro de Física de Materiales CSIC, UPV/EHU, Spain)
Dr. Jorge Kohanoff (Queen's University of Belfast, UK)
Dr. José Miguel Pruneda (Instituto de Ciencia de Materiales de Barcelona ICMAB-CSIC, Spain)
Dr. Daniel Sánchez-Portal (DIPC, Centro de Física de Materiales CSIC, UPV/EHU, Spain)

The workshop aimed to be a platform for interaction between expert theoretical and experimental scientists working in the field of the radiation damage at the atomic scale. The program of this 3-day workshop was built around a number of invited talks covering some important recent contributions to the field and poster sessions.

Scientific Objectives
The objective of this event was to get together experts in the field of radiation damage in materials, with special attention to the challenges for a microscopic theoretical description of the many processes involved in the radiation damage of real materials. In particular, great emphasis was placed on the study of the energy transfer processes between fast projectiles and the electrons in the target material. The influence of such excited hot electrons in the dynamics of the atoms of the target and other non-adiabatic effects will be considered in detail. The most relevant experimental aspects of the field was also covered by renowned experts.

CONTRIBUTIONS

Prof. Fernando Agulló-López (Universidad Autónoma de Madrid, Spain)
Damage and amorphization induced by swift-ion beams: A non-radiative exciton model

Prof. Andrés Arnau (Basque Country University CSIC-UPV/EHU, San Sebastián, Spain)
How far can we go with jellium models to describe valence electron excitations in solids?

Prof. Peter Bauer (Institute of Experimental Physics, Johannes Kepler University, Linz, Austria)
Electronic stopping of slow light ions in materials with large band gaps: an experimental approach

Prof. Alfredo Caro (Los Alamos National Laboratory, Los Alamos, USA)
Modeling collision cascades in metals: 25 years after

Prof. Alfredo Correa (Lawrence Livermore National Laboratory, California, USA)
Time-dependent DFT Simulations of Electronic Stopping

Prof. Christian Dufour (Centre de Recherche sur les Ions, les Matériaux et la Photonique, Caen, France)
Matter transformation by swift heavy ions: a thermodynamic point of view

Dr. Daniel Dundas (Queen's University of Belfast, Belfast, UK)
Correlated electron-ion dynamics in atomic wires

Prof. Marie-Pierre Gaigeot (Université d'Evry, France)
TD-DFT MD investigation of the ultrafast dissociation of ionised biomolecules immersed in water: direct and indirect chemical reactivity

Prof. Rafael García-Molina (Universidad de Murcia)
Monte Carlo Modelling of Charged Particle Transport in Biological Materials Using a Dynamic Non-local Target Energy-Loss Function

Dr. Arkady Krasheninnikov (University of Helsinki and Helsinki University of Technology, Helsinki, Finland)
Irradiation effects in carbon and boron-nitride nanostructures: an insight from atomistic simulations

Dr. Christian Linsmeier (Max-Planck-Institut für Plasmaphysik, Garching, Germany)
Ion-induced surface chemistry in materials for fusion first wall applications

Dr. Daniel Mason (Imperial College London, UK)
Non-adiabatic forces on ions in radiation damage in metals

Dr. Jorge A. Morales (Texas Tech University, USA)
The Electron Nuclear Dynamics Theory and Related Models: from Ion-Molecule Collisions to Classical Charge-Equilibration Models

Prof. Thomas M. Orlando (School of Chemistry and Biochemistry, Georgia Tech, USA)
The role of resonances and diffraction in electron-beam induced damage of DNA and RNA thin-film targets

Dr. Chris Race (Imperial College London, UK)
Large scale semi-classical simulations of ion channelling with time-dependent tight-binding

Dr. Thomas Schlathölter (University of Groningen, The Netherlands)
Photodissociation and ion-induced dissociation of complex biomolecules

Prof. Eric Suraud (Université Paul Sabatier, Toulouse, France)
Towards the microscopic description of the irradiation of biomolecules

Prof. Francois Willaime (CEA Saclay, France)
DFT energy landscape of radiation defects in metals for kinetic models

PASSION FOR **PHOTONS**

2010

September 29 - October 1, 2010

ORGANIZERS
Ricardo Diez Muiño Passion for Knowledge: The Workshops
Javier Aizpurua Passion for Photons

Addressing fundamental and applied aspects of nanoscale optics.

CONTRIBUTIONS

Keynote: Passion for Photons
Prof. Naomi Halas (Rice University, Houston, USA)
Plasmonics: nanoscale manipulation of light

Nanoantennas

Prof. Lukas Novotny (University of Rochester, USA)
Nonlinear plasmonics with optical antennas

Dr. Garnett Bryant (NIST, Gaithersburg, USA)
Photonics with nanohybrids

Francesco De Angelis (Italian Institute for Technology, Genova, Italy)
Plasmon polariton nanotantenna for single molecule detection

Keynote: Passion For Soft Matter
Prof. Dieter Richter (Forschungszentrum Jülich, Germany)
Soft Matter and Live Science: Research with Neutrons

Concepts in Optics

Prof. Sir John Pendry (Imperial College London, UK)
Transformation Optics at Optical Frequencies

Prof. Shiwu Gao (University of Göteborg, Sweden)
Insights on surface plasmons from quantum mechanics

Antonio García-Martín (Inst. de Microelectrónica de Madrid, CSIC Spain)
Active magnetoplasmonics in hybrid metal/ferromagnet/metal microinterferometers

Keynote: Passion for Interfaces
Prof. Fernando Flores (UAM, Madrid, Spain)
Organic and inorganic semiconductor interfaces across physics, chemistry and time

Electrons and Photons

Prof. Archie Howie (University of Cambridge, UK)
Photons and electrons: Tightening their embrance

Prof. F.J. García de Abajo (Institute of Optics CSIC, Madrid, Spain)
Photons and electrons team up

Dr. Alejandro Reyes Coronado (IESL-FORTH, Heraklion, Greece)
Plasmonic forces induced by electrons

Coherence and Fast Control

2010

Prof. Peter Nordlander (Rice University, UK)
"Fano resonances in plasmonic nanostructures

Prof. Mark Stockman (Georgia State University, Atlanta, USA)
Trends in Nanoplasmonics: Ultrasmall, Ultrafast, Ultrastrong

Dr. Otto Muskens (University of Southampton, UK)
Active plasmonic nanoantennas for optical switching

Dr. Ricardo Sapienza (ICFO, Barcelona, Spain)
LDOS fluctuations probed by single-molecule spectroscopy in random and periodic media

Taking Advantage of the Near_Field

Dr. Rainer Hillenbrand (nanoGUNE, San Sebastian, Spain)
Scattering-type Scanning Near-Field Optical Microscopy

Dr. Riedel Damien (Nanophysics Lab. CNRS, Orsay, France)
A scanning tunneling microscope as a tunable nanoantenna for atomic scale control of optical-field enhancement

Dr. M.L. Juan (ICFO, Barcelona, Spain)
Self-induced back-action optical trapping

Dr. Amador Menéndez (Instituto tecnológico de Materiales de Asturias, Spain)
Improving the efficiency of luminescent solar concentrators

Theory
Prof. Nader Engheta (University of Pennsylvania, USA)
From Electronics to Metatronics to Graphene Metamaterials

Prof. F. J. García Vidal (Universidad autónoma de Madrid, Spain)
Controlling the flow of surface plasmons

PASSION FOR **PHOTONS**

Prof. Juan José Sáenz (Universidad autónoma de Madrid, Spain)
Resonant optical forces on metallic and dielectric nanoparticles

Prof. Fernando Moreno (Universidad de Cantabria, Santander, Spain)
Electromagnetic interactions between plasmon nanostructures and substrates

Plasmon-Bio-nanosense (Session sponsored by ESF)

Dr. Romain Quidant (ICFO, Barcelona, Spain)
Plasmon nano-optics: designing novel nanotools for Biosciences and Medicine

2010

Prof. Mikael Kall (Chalmers University of Technology, Sweden)
Nanoplasmonic sensing: refractive index, SERS and optical forces

Prof. J.R. Krenn (University of Graz, Austria)
Plasmonic control of elementary emitters

Dr. Jaime Gómez Rivas (AMOLF, The Netherlands)
Collective plasmonic resonances in arrays of nanoantennas

Prof. Luis Martin-Moreno (Inst. de Ciencia de Mat. de Aragón, Spain)
Extraordinary optical transmission due to strongly localized modes

Alberto Curto (ICFO- Barcelona, Spain)
A nano-optical Yagi-Uda antenna driven by a quantum dot

Plasmon Bio-nanosense (Session sponsored by ESF)

Prof. Stefan Maier (Imperial College London, UK)
Correlative electron and optical spectroscopies of metallic nanostructures and applications in anometrology

Dr. Andrea Csáki (IPHT, Jena, Germany)
Plasmonic-tuned microstructured optical fibers for localized surface plasmon resonance (LSPR) sensing

Bjoern Niesen (IMEC vzw, Leuven, Belgium)
Interactions of excitons with localized surface plasmons in organic semiconductor-metal nanoparticle thin-films

Antonio Fernández (Imperial College London, UK)
Kissing spheres: broadband response and superfocusing properties

Number of participants: 83

PASSION FOR KNOWLEDGE

The Workshops

PASSION FOR **INTERFACES**

September 28-30, 2010

ORGANIZERS
Ricardo Diez Muiño Passion for Knowledge: The Workshops
Maite Alducin Passion for Interfaces

Unraveling fundamental aspects of the scattering and reactivity of atoms and molecules at interfaces, electronic properties of thin films and adsorbates, self-assembling and surface functionalization.

2010

CONTRIBUTIONS

Keynote Lecturer: F. Flores (UAM, Madrid, Spain)
Organic and inorganic semiconductor interfaces across physics,chemistry and time

Chairman: Prof. Martin Weinelt (Freie Universität, Berlin, Germany)

Keynote: Passion for Electrons
Prof. W-D Schneider (École Polytechnique Fédérale de Lausanne)
Quantum oscillations, superconductivity, zero-bias anomalies, and Coulomb blockade in nanoscaled supported lead islands

Chairman: Prof. Geert-Jan Kroes (Leiden University, Netherlands)

Prof. Miquel Salmeron (LBNL and University of California, USA)
From vacuum to atmosphere: microscopies and spectroscopies for molecular level studies of surfaces and interfaces

Prof. Emilio Artacho (University of Cambridge, UK)
First-principles simulations of oxide hetero-structures: electrostatics, interface charges and vacancies

Prof. Hajo Freund (Fritz Haber Institute, Germany)
Electronic structure relations of oxide metal interfaces at the atomic level

Chairman: Prof. Hajo Freund (Fritz Haber Institute, Germany)

Prof. Rodolfo Miranda (IMDEA and UAM, Madrid, Spain)
Periodically Rippled Epitaxial Graphene: An Electronically and Structurally Nanostructured Material

Dr. Daniel Sánchez-Portal (CFM, San Sebastián, Spain)
Graphene interacting with transition metals: tuning the electronic and magnetic properties of graphene

2010

Dr. E. Avellar Soares (Physics Department-ICEx-UFMG, Brazil)
Graphene-covered iron layers on Ni(111): structural and electronic properties

Dr. Laura Fernández (DIPC, Spain)
Ultra-high dense array of magnetic quantum dots on a GdAu2 template

Chairman: Prof. Antoine Salin (Université Bordeaux, France)

Prof. Aart Kleyn (FOM Institute, Nieuwegein, Netherlands)
When energy is not a problem: interactions with fast and excited particles at surfaces

Dr. Pascal Larregaray (CNRS/Université Bordeaux1, France)
Theoretical investigation of the Eley-Rideal recombination of nitrogen on W(100)

Dr. Serge Monturet (Universität Potsdam, Germany)
Electronic damping of vibrations: the case of NO on Au(111)

Chairman: Dr. Javier Aizpurua (CFM and DIPC, San Sebastián, Spain)

Keynote: Passion for Photons
Prof. Naomi Halas (Rice University, Houston, USA)
Plasmonics: nanoscale manipulation of light

Chairwoman: Prof. Maki Kawai (RIKEN, Wako, Japan)

Prof. Karina Morgenstern (Leibniz Universität, Hannover, Germany)
Single molecule manipulation by light and electrons

Prof. Karsten Reuter (TU, München, Germany)
Adsorption of aromatic molecules: Tackling the van der Waals challenge with DFT-D?

Chairman: Prof. Juan Colmenero (UPV-CFM and DIPC, San Sebastián, Spain)

Prof. Dieter Richter (Forschungszentrum Jülich, Germany)
Soft Matter and Live Science: Research with Neutrons

Chairman: Prof. Aart Kleyn (FOM Institute, Nieuwegein, Netherlands)

Dr. Celia Rogero (CFM, San Sebastián, Spain)
Surface coordination chemistry: structure and reactivity of tetrapyrrole molecules

Dr. H. Fabio Busnengo (Universidad Nacional de Rosario, Argentina)
Structure of self-assembled monolayers of alkylthiolates on Au(111) and Ag(111): a comparative study based on Density Functional and post Hartree-Fock calculations

2010

Maria J.T.C. van der Niet (Leiden University, Netherlands)
Interactions between H2O and pre-adsorbed O or D on stepped platinum surfaces
Chairman: Dr. Ricardo Díez Muiño (CFM and DIPC, San Sebastián, Spain)

Prof. Fernando Flores (UAM, Madrid, Spain)
Organic and inorganic semiconductor interfaces across physics, chemistry and time

Chairman: Prof. Andrés Arnau (UPV- CFM, San Sebastián, Spain)

Prof. Maki Kawai (RIKEN, Wako, Japan)
Single Molecule Spectroscopy: Electronic state, vibrational state and spin state

Prof. Pietro Gambardella (CIN2, Barcelona, Spain)
Spin-spin and spin-orbital coupling effects at metallic interfaces

Dr. Lucia Vitali (CFM and UPV, San Sebastián, Spain)
Potential barrier mapping at metal-organic nanocontacts

Chairman: Prof. Enrique Ortega (UPV- CFM, San Sebastián, Spain)

Prof. Franz J. Himpsel (University of Wisconsin Madison, USA)
Atom-Specific Spectroscopy of Interfaces for Biosensors and Solar Cells

Dr. Nicolás Lorente (CIN2, Barcelona, Spain)
Mixed-valency signature in vibrational inelastic electron tunneling spectroscopy

Prof. J. I. Pascual (Freie Universität, Berlin, Germany)
Charging and electric field gating individual molecules at a hybrid metal-organic interface

Dr. Aitor Mugarza (CIN2, Barcelona, Spain)
Exotic Kondo effect in metalorganic complexes controlled by ion-substrate interaction

Chairman: Prof. Emilio Artacho (University of Cambridge, UK)

Prof. G. -J. Kroes (Leiden University, Netherlands)
Achieving chemical accuracy for a prototype molecule-surface reaction

Dr. Holly Hedgeland (University of Cambridge, UK)
Dynamic and static processes in interface interaction

Jörg Meyer (Fritz-Haber Institute, Berlin, Germany)
QM/Me – a novel embedding approach for adsorbate dynamics on metal surfaces

Gerson Mette (Philipps-Universität, Marburg, Germany)
Time-resolved investigation of laser-induced diffusion by optical second-harmonic microscopy

Number of participants: 86

PASSION FOR KNOWLEDGE

The Workshops

PASSION FOR SOFT MATTER

2010

September 28-30, 2010

ORGANIZERS

Ricardo Diez Muiño Passion for Knowledge: The Workshops
Arantxa Arbe Passion for Soft Matter

Presenting state-of-the-art experiments and theoretical advances in the fields of soft matter (polymers, colloids, amphiphiles, biomaterials and composites).

CONTRIBUTIONS

Keynote Lecturer: D. Richter (Forschungszentrum, Jülich, Germany)

Keynote: Passion for Electrons
Chair: Prof. Martin Weinelt (Free University Berlin, Germany)

Prof. T.W. Hänsch (MPI, Garching, Germany)
Keynote Passion for Electrons

Novel Materials
Chair: Prof. José A. Pomposo (Centro de Física de Materiales UPV/EHU-CSIC and Ikerbasque, Spain)

Prof. Thomas P. Russell (University of Massachusetts Amherst, USA)
Directed Self-Assembly of Block Copolymers over Macroscopic Length Scales

Prof. Ralph H. Colby (The Pennsylvania State University, USA)
Designing Ion-Containing Polymers for Facile Ion Transport

Prof. Theyencheri Narayanan (ESRF, France)
Probing the multi-level structure and dynamics of soft matter using X-ray scattering

Confined Water
Chair: Dr. Silvina Cerveny (Centro de Física de Materiales UPV/EHU-CSIC, Spain)

Prof. Feri Mezei (ESS Collaboration, Lund, Sweden and Hungarian Academy of Sciences, RISSP, Budapest)
Study of Nanoscale Protein Dynamics by High Power Neutron Spectroscopy

Prof. Fabio Bruni (Universitá di Roma Tre, Italy)
Water near proteins and under confinement: is that a good model for bulk water?

Prof. Paola Gallo (University Roma Tre, Italy)
Water and The Others: Simulations of Supercooled Water in Confinement and Solutions

Dr. Sandrine Lyonnard (CEA, France)
The dynamical behaviour of water confined in perfluorinated ionomers and surfactants

Window to Biology
Chair: Prof. Rod Quirk (University of Akron, USA)

Prof. Jan Skov Pedersen (University of Aarhus, Denmark)
The Structure of Protein-Detergent Complexes from Small-Angle X-ray Scattering

Dr. Ilja Voets (Adolphe Merkle Institute, University of Fribourg, Switzerland)
Complex Polymer Assemblies

Prof. Dmitry Matyushov (Arizona State University, USA)
Electrostatics and viscoelasticity of protein-water interface

2010

Keynote: Passion for Photons
Chair: Dr. Javier Aizpúrua (Centro de Física de Materiales UPV/EHU-CSIC and DIPC, Spain)

Prof. Naomi Halas (Rice University, Houston, USA)
Keynote Passion for Photons

Emerging Properties
Chair: Prof. Jörg Baschnagel (Institut Charles Sadron, France)

Prof. Pablo G. Debenedetti (Princeton University, USA)
Thermodynamic and Kinetic Models of the Emergente of Biochemical Homochirality.

Prof. Francesco Sciortino (Universitá di Roma La Sapienza, Italy)
Self Assembly of Janus Particles and other Patchy Colloids

Keynote: Passion for Soft Matter
Chair: Prof. Juan Colmenero (Centro de Física de Materiales UPV/EHU-CSIC and DIPC, Spain)

Prof. Dieter Richter (Forschungszentrum Jülich, Germany)
Soft Matter and Live Science: Research with Neutrons

Dynamic Asymmetry, Viscoelastic Phase Transitions
Chair: Prof. Carmen Mijangos, Instituto de Ciencia y Tecnología de Polímeros, CSIC, Spain)

Prof. Hajime Tanaka (University of Tokyo, Japan)
Pattern evolution - From viscoelastic phase separation to mechanical fracture

Dr. Satoshi Koizumi (Japan Atomic Energy Agency, Japan)
Dynamic Asymmetry Effects on Soft-Matters: Small-angle Scattering Studies of Their Rich Varieties Ranging from Viscous-to-Gel Limits

Dr. Laurence Noirez (Laboratoire Léon Brillouin, France)
Hidden Macroscopic Shear Elasticity in Viscous Liquids

PASSION FOR **SOFT MATTER**

Keynote: Passion for Interfaces
Chair: Prof. Antoine Salin, Université Bordeaux, France)

Prof. Fernando Flores (UAM, Madrid, Spain)
Organic and inorganic semiconductor interfaces across physics, chemistry and time

Dynamics at Different Scales
Chair: Dr. Daniele Cangialosi, Centro de Física de Materiales UPV/EHU-CSIC, Spain)

Prof. Alexei P. Sokolov (University of Tennessee, USA)
Decoupling phenomena in dynamics of Soft Matter: From small molecules to proteins

Prof. Kenneth S. Schweizer (University of Illinois at Urbana-Champaign, USA)
Slow Dynamics in Soft Glassy Materials

Prof. Vladimir Novikov (University of Tennessee, USA)
Influence of pressure on fast relaxation in glass-forming materials

Self-Assembled Systems
Chair: Dr. Gustavo Schwartz, Centro de Física de Materiales UPV/EHU-CSIC, Spain)

Prof. Angel Alegría (Centro de Física de Materiales UPV/EHU-CSIC, Spain)
Structure - dynamics relationship in nano-structured diblock-copolymers by dielectric spectroscopy

Prof. Christiane Alba Simionesco (CEA Saclay, France)
How anomalous remain the liquid water properties when it is confined at the nanoscale?

Dr. Reidar Lund (DIPC, San Sebastián, Spain)
Non-equilibrium Kinetics in Block Copolymer Micelles

Prof. Soren Toxvaerd (Roskilde University, Denmark)
Crystallization of supercooled nanodroplets

Dynamics Of Polymers In Different Environments
Chair: Dr. Fernando Alvarez, Centro de Física de Materiales UPV/EHU-CSIC, Spain)

Dr. Angel Moreno (Centro de Física de Materiales UPV/EHU-CSIC, Spain)
Computer simulations of polymer blends: from structural relaxation to caín dynamics

Dr. Jörg Baschnagel (Institut Charles Sadron, France)
Deviations from Chain Ideality in Polymer Melts

Dr. Apostolos Kyritsis (National Technical University of Athens, Greece)
Dynamic heterogeneity in binary poly(ethyl acrylate) /p-xylene mixtures

Dr. Nigel Clarke (Durham University, UK)
Dynamics in polymer nanocomposites

Number of participants: 103

PASSION FOR KNOWLEDGE

The Workshops

PASSION FOR **ELECTRONS**

September 28-30, 2010

ORGANIZERS
Ricardo Diez Muiño Passion for Knowledge: The Workshops
Vyacheslav M. Silkin Passion for Electrons

Advances in ultrafast dynamics, attosecond physics, electronic excitations in solids, nanostructures and other low-dimensional systems.

CONTRIBUTIONS

SEPTEMBER 28

Keynote Lecturer: W-D. Schneider (École Polytechnique Fédérale de Lausanne, Switzerland)
Quantum oscillations, superconductivity, zero-bias anomalies, and Coulomb blockade in nanoscaled supported lead islands

Prof. J. Kirschner (Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany)
Experiments on the exchange-correlation hole in solids

Prof. F. Martin (Universidad Autónoma de Madrid, Spain)
Electron Localization following Attosecond Molecular Photoionization of H2

Prof. D. Menzel (Fritz-Haber-Institut der MPG, Berlin, Germany)
NO photochemistry on silver nanoparticles by nanosecond vs. femtosecond excitation

Prof. S. Blügel (Forschungszentrum, Julich,Germany)
Electrons at surfaces: From Rashba effect to topologically protected spin textures

Prof. J.P. Gauyacq (Université Paris-Sud, Orsay, France)
Magnetic transitions induced by tunnelling electrons in individual adsorbates

Dr. J. Fransson (Uppsala University, Sweden)
Dynamical exchange interaction between localized spins in nonequilibrium

Prof. H.Ch. Schneider (TU, Kaiserslautern, Germany)
Ultrafast demagnetization dynamics in ferromagnets and Heusler alloys

Prof. R. Kienberger (Max-Planck-Institut für Quantenoptik, Garching, Germany)
Attosecond spectroscopy on solid surfaces

Prof. A.K. Kazansky (Fock Institute of Physics, Sankt Petersburg, Russia)
Some aspects of the theory of streaking experiments with subfemtosecond pulses on solids

Dr. Ch. Lemell (Vienna UT, Austria)
Modelling XUV-NIR streaking experiments at metal surfaces

SEPTEMBER 29

Keynote: Passion for Photons
Prof. N. Halas (Rice University, Houston, USA)
Plasmonics: nanoscale manipulation of light

Prof. M. Rocca (Universitá di Genova, Italy)
Acoustic Surface Plasmons, a novel collective excitation at metal surfaces, with promising applications

Prof. T. Nagao (National Institute for Material Science, Tsukuba, Japan)
Plasmon propagation and confinement in atom-scale chains and sheets

Keynote: Passion for Soft Matter
Prof. D. Richter (Forschungszentrum Jülich, Germany)
Soft Matter and Live Science: Research with Neutrons

Prof. U. Höfer (University of Marburg, Germany)
Coherent dynamics of image-potential electrons

Prof. A. Rubio (University of the Basque Country, San Sebastián, Spain)
First principle modeling of the excited state properties of complex nanostructures and biomolecules: a TDDFT and Many-Body perturbation theory approach

Dr. J. Stähler (Fritz-Haber-Institut der MPG, Germany)
Ultrafast dynamics of coherent phonons during the insulator-metal transition of VO2

SEPTEMBER 30

Keynote: Passion for Interfaces
Prof. F. Flores (UAM, Madrid, Spain)
Organic and inorganic semiconductor interfaces across physics,chemistry and time

Prof. H. Petek (University of Pittsburg, USA)
Imaging the femtosecond time scale correlated electron-nuclear dynamics in surface photodesorption

Prof. E.V. Chulkov (University of the Basque Country, San Sebastián, Spain)
Decay mechanisms of single particle excitations in nanostructures surfaces

Prof. A. Heidenreich (University of the Basque Country, San Sebastián, Spain)
Laser pulse length dependence of electron and nuclear dynamics in Coulomb explosions of xenon clusters

Prof. M. Aeschlimann (University of Kaiserslautern, Germany)
Lifetime of optically excited electrons

Prof. B. Gumhalter (Institute of Physics, Zagreb, Croatia)
Ultrafast electron dynamics in pump-probe spectroscopies of surfaces: from transient excitonic to quasi-stationary polaronic states

Prof. J.M. Pitarke (CICnanoGUNE, San Sebastián, Spain)
The asymptotic behavior of the Kohn-Sham potential of Density-Functional Theory at metal surfaces

Prof. V.U. Nazarov (RCAS, Academia Sinica, Taipei, Taiwan)
Performance of the exchange-correlation kernel of time-dependent density-functional theory derived from LDA to to current-density functional theory

Prof. Ph. Hofmann (University of Aarhus, Denmark)
The electronic structure of graphene: confinement-induced band gap opening and core electrón delocalization

Prof. A.A. Lucas (FUNDP, Nandrin, Belgium)
Plasmon tsunami on C60 caused by electron transfer to a highly charged ion

Dr. L. Chico (Instituto de Ciencia de Materiales CSIC, Madrid, Spain)
Interface states in carbon nanotube junctions: Rolling up graphene

Dr. J. Zhao (University of Pittsburgh, USA)
The electronic structure graphane and graphane nanostructures from ab initio theory

Number of participants: 78

European Physical Society Committee Meeting

October 1-2, 2010

CONTRIBUTORS

Carlos Hidalgo Plasma Physics Division
Bob Lambourne Physics Education
Jan Mostowski EPJ
M. Rosario Héras Celamin Royal Spanish Physical Society
Maria Helena Nazar Portuguese Physical Society
Igor Campillo Passion for Knowledge
Pedro Miguel Echenique Landiribar DIPC

2010

JCNS Panel Meeting

November 29-30, 2010

ORGANIZER
Arantxa Arbe (DIPC, Spain)

DIPC hosted the meeting of the JCNS Panel for proposals selection. After the permanent shut down of the research reactor FRJ-2 in Jülich, the Jülich Centre for Neutron Science (JCNS, http://www.jcns.info) has been founded. It encompasses the in-house research of the Institut für Festkörperforschung Jülich with neutrons, the instrument and method development and the instrument operation and user programs at the FRM-II reactor in Munich, the SNS Spallation Source in Oak Ridge and the ILL high-flux reactor in Grenoble. Twice a year, a committee of external experts in neutron scattering selects the best proposals from those submitted from allover the world to grant beamtime in the different instruments. In the November meeting celebrated at the DIPC 134 proposals were discussed. The Panel consists of a Chairperson (A. Arbe, CFM, San Sebastián) and 10 members (Stephan Förster, Bernhard Frick, Kim Lefmann, Roland May, Julian Oberdisse, Frederic Ott, Christian Pfleiderer, Walter Richtering, Henrik Rønnow, Kristiaan Temst, and Regine Willumeit). In addition, two representative persons from JCNS (Alexander Ioffe and Thomas Gutberlet) attended the meeting to inform the Panel about the state of the art and future development of the instruments.

Symposium on Surface Science

March 6-12, 2011
Baqueira Beret, Lleida, Spain

ORGANIZERS
Andrés Arnau (UPV/EHU, CFM, DIPC, Spain)
Pedro M. Echenique (UPV/EHU, CFM, DIPC, Spain)

CONTRIBUTIONS

Chairperson Wolf-Dieter Schneider

Michael Altman
Moiré Twist in Graphene on Ru(0001)

2011

Chairperson Pedro Miguel Echenique

Dietrich Menzel
Ultrafast charge transfer at graphene surfaces

Norbert Müller
Interplay between Electronic correlations and Coherent Structural Dynamics during the Monoclinic Insulator-to-Rutile Metal Phase Transition in VO2

Ulrich Höfer
Time-resolved two-photon photoemission of metal/organic interface states

Wolf Widdra
Electronic properties of NiO thin films: A combined STM, STS, and 2PPE study

---

Chairperson U. Diebold

Claudia Ambrosch-Draxl
A Growth Model Based on Experiments and Simulations

Armin Gölzhäuser
Janus nanomembranes: Surfaces without bulk, functionalized on both sides

Manfred Buck
Electrochemical Generation of Low Dimensional Metal Structures on Top of Self-Assembled Monolayers

Christof Wöll
Charge Transport Through and Within Self-Assembled Monolayers: New Insights from Nanofabricated Model Devices

---

Chairperson F. Netzer

Matthias Scheffler
Gold clusters at finite temperature in vacuo and in a CO plus O2 atmosphere: ab initio studies towards gold catalysis

Geoff Thornton
Defects on room temperature ultra-thin film CeO2 with STM

Chairperson E. Lundgren

Peter Varga
High Island Densities in Pulsed Laser Deposition: Causes and Implications

Yuriy Yanson
Copper electrodeposition on fast time scale: from underpotential deposition to bulk growth

Phil Willmott
Buckling under tension – LaAlO3 on SrTiO3

Fabien Cheynis
Dewetting dynamics of crystalline thin films

Chairperson M. Scheffler

Pascal Ruffieux
On-surface synthesis and characterization of grapheme nanostructures

Gustavo Ceballos
Growth of graphene nanoislands on a Ni(111) surface

Goucai Dong
Kinetics of graphene growth on Rh(111)

Gilberto Teobaldi
Structure and properties of surface and subsurface defects in graphite accounting for van der Waals and spin polarization effects

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Chairperson G. Thornton

Ulrike Diebold
STM investigations of pure and Sn-doped In2O3 surfaces

Falko Netzer
Fabrication of a NiOx nanodot superlattice

Chairperson F. Himpsel

Aitor Mugraza
Tuning the magnetic moment of individual molecules at the metallic interface

Ulrich Heinzmann
Spin-resolved Photoelectron Spectroscopy of Mn6Cr Single-Molecule-Magnets and of Manganese Compounds as Reference Layers

Daniel Sánchez Portal
Magnetism of Covalently Functionalized Graphene

Poster presentations

Chairperson H. Brune

M. Faraggi
Characterization of an oxalic acid layer on Cu(111)

Q. Liu
Study of NO reduction by H2 on a Pt(110) model catalyst in a High-Pressure STM

V.M. Silkin
Ultrafast screening of a point charge at a metal surface

A. García-Lekue
Plane-wave based Electron Tunneling trough Au Nanojunctions

S.J. Leake
Structural studies of the metal-insulator transition in LaNiO3 thin films

N. Gonzalez Lakunza
Structure and electronic properties of TCNQ-F4 deposited on clean Au(111)

M. Dürr
Fast and with atomic precision – real-space investigation of hydrogen diffusion on Si(001) using nanosecond laser heating and STM

V. Navarro
Cobalt catalyst in action followed at high pressures with STM and SXRD during hydrocarbon synthesis

S. Blomberg
The high pressure oxidation and reduction by CO of Rh – from single crystal to nanoparticles

P. Cabrera-Sanfelix
Water Adsorption on Clean and Oxygen Decorated Metal Substrates

Johannes V. Barth
Assembly and manipulation of supramolecular dynamers and rotatable sandwich complexes on a surface

Ulrich Heinzmann
Preparation of Monolayers of Mn6Cr Single Molecule-Magnets on different Substrates and characterization by means of nc-AFM

T. Passanante
Thermal decomposition of oxidised Silicon-on-insulator thin film

M. E. Messing
Generation of Pd model catalyst nanoparticles by spark discharge

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Chairperson E. Taglauer

F. Aumayr
Nano-craters formed by impact of individual highly charged ions on PMMA surfaces

P. Bauer
Information depth in Low Energy Ion Scattering

Chairperson D. Menzel

F. J. Himpsel
Magnetism at Stepped Silicon Surfaces

J. I. Cerdá
CoPc adsorption on Cu(111): Origin of the C4 to C2 symmetry reduction

E. V. Chulkov
Electronic structure of topological insulators

J. E. Ortega
Tailoring interactions in supramolecular networks by fluorination

---

Chairperson Pascal Ruffieux

W.D. Schneider
Supramolecular self-assembly driven by electrostatic repulsion:
The 1D aggregation of Rubrene pentagons on Au(111)

K. Morgenstern
Preferred Pathway for a Molecular Photo Switch inContact with a Surface

H. Daimon
Wide acceptance angle photoelectron spectrometer for stereophotograph of atomic arrangement

E. Lundgren
Probing a surface reconstruction with anomalous X-ray diffraction

---

Chairperson K. Morgenstern

T. Stempel
Bridging the Pressure Gap -
Developments and Challenges for Ambient Pressure Photoelectron Spectroscopy

M. Maier
High Precision local electrical Probing at T< 5K: Potential and Limitations for the Analysis of Nanocontacts and Nanointerconnects

---

Chairperson F. Aumayr

T. Koshikawa
Dynamic magnetic domain observation with novel highly spin polarized and high brightness LEEM

J. Gustafson
Methane oxidation over Pd and Pt: linking surface science and industrial catalysis

S. Yu. Krylov
Atomic scale friction: Physically nontrivial problems

F. Salvat-Pujol
Contribution of surface excitations to secondary-electron emission observed by secondary-electron-energy-loss coincidence spectroscopy

---

Chairperson P. Muller

D. Stradi
The role of dispersion forces in the structure of grapheme monolayers over the Ru(0001) surface

F. Tabak
Fast scanning with piezo/counter-piezo elements and MEMS scanners: a comparison

F. J. Giessibl
Sensing Atomic Forces

T. Frederiksen
Atomic-scale engineering of electrodes for single-molecule contacts

Highlights in Quantum Condensed Matter Physics

June 17-23, 2011

ORGANIZERS
F. Sebastian Bergeret (CFM-CSIC, DIPC, Donostia-San Sebastián, Spain)
Miguel A. Cazalilla (CFM-CSIC, DIPC, Donostia-San Sebastián, Spain)
Chandra M. Varma (University of California Riverside, USA)
F. (Paco) Guinea (Instituto de Ciencia de Materiales de Madrid-CSIC, Spain)

The aim of this workshop was to bring together leading researchers working at the frontier of Condensed Matter Physics, in topics which include Graphene and Topological Insulators, High-Tc Superconductivity, Superconductivity at the Mesoscale, and Ultracold Atomic Gases.

CONTRIBUTIONS

Topological Insulators and Topological Phase Transitions
Laurens Molenkamp (Würzburg): Dirac Fermions in HgTe Quantum Wells.
Frederik Schiller (San Sebastian): Lifshitz Transition at the Surface of Noble Metals.

High-Tc Superconductivity (I)
Zhi-Xun Shen (Stanford): Dynamic Gap Competition Leading to a Revised Cuprate Phase Diagram
Steven Kivelson (Stanford): Aspects of the Phase Diagram of the Hubbard Model
Welcome Address by the President of DIPC Pedro M. Echenique

High-Tc Superconductivity (II)
Philippe Bourges (Saclay): Novel Magnetic Order and Excitations in High-Tc Copper-oxide Superconductors
Vivek Aji (Riverside): Quantum Criticality in Dissipative Quantum
Two-Dimensional XY and Ashkin-Teller Models: Application to the Cuprates

One Dimensional Systems and Beyond
Leonid Glazman (Yale): Non-linear Quantum Liquids in One Dimension
Julia Meyer (Grenoble): Phase Transitions in Quantum Wires
Masaki Oshikawa (Tokyo): Frequency Shift of Electron Spin Resonance
Thierry Giamarchi (Geneva) Spin Dimers: From BEC to Luttinger Liquids
Fractional Quantum Hall Effect and Topological Quantum Computing
F. Duncan Haldane (Princeton):
Hall Viscosity and A New Geometric Description of the Fractional Quantum Hall Effect
Inés Safi (Orsay): Measuring Fractional Charges without Recourse to Noise: A Novel Proposal
Yuval Oreg (Weizman): Majoranas and Topological Quantum Processing in 1D Networks
Daniel Arovas (San Diego): Gamma Matrix Generalizations of the Kitaev Model

Graphene and Graphene-related Phenomena (I)
Jennie Lau (Riverside): Quantum Transport in Suspended Bilayer and Trilayer Graphene
José González (Madrid): Higgs-like Condensation of Ripples and Buckling Transition in Graphene
Pablo Jarillo-Herrero (MIT): Electronic Transport in Graphene and Topological Insulators
Maxim Kharitonov (Rutgerts): Correlated º = 0 Quantum may States in Mono- and Bilayer Graphene

Graphene and Graphene-related Phenomena (II)
María Vozmediano (Madrid): Aharonov-Bohm Interference from Local Deformations in Graphene
Michael Fogler (San Diego): Graphene Nanoplasmonics
Alexey Nikitin (Zaragoza): Nanoemitters in Graphene

Strong Correlations in Ultracold Gases and Condensed Matter(I)
Christophe Salomon (Paris): Quantum Simulation of Strongly Correlated Fermions with Cold Atomic Gases
Marco Polini (SNS Pisa): Spin Dynamics and Spin Drag in Fermi Gases
Konstantin Efetov (Bochum): Describing Systems of Interacting
Fermions by Boson Models: Mapping in Arbitrary Dimension and Applications
AlejandroMuramatsu (Stuttgart): Correlated Fermions on Graphenelike Lattices

Strong Correlations in Ultracold Gases and Condensed Matter (II)
Sungkit Yip (Academia Sinica): Spinor Bosons in Optical Lattices
Shan-Wen Tsai (Riverside): Mediated Interactions and Correlated Phases in Cold Atom Mixtures
Frank Hekking (Grenoble) Persistent Currents in a One-dimensional Bosonic Ring

Topologically Ordered Matter
Shoucheng Zhang (Stanford): Topological Insulators and Superconductors
Aharon Kapitulnik (Stanford): STM Studies of the Local Density of States Near Impurities and
Macroscopic Defects on the Surface of Topological Insulators
Leon Balents (Santa Barbara): Quantum Spin Liquids in Quantum Spin Ice
Tero Heikkil¨a (Helsinki): High Temperature Surface Superconductivity in Topological Flat Band Systems

High-Tc Superconductivity (III)
Greg Boebinger (Florida): Heat Capacity of Underdoped YBCO through the
Magnetic-field-induced Resistive Transition: d-wave Superconductor Or Fermi Liquid Or Both Or Neither
Chandra Varma (Riverside) Pseudogap State of the Cuprates
Jörg Schmalian (Karlsruhe): Ising-nematic Order in the Ironbased Superconductors
Piotr Chudzinski (Geneva): Collective Excitations and Tow Temperatura Transport Properties of Bismuth
Javier Sanchez-Yamagishi (MIT): Quantum Hall Effect and Screening in Twisted Bilayer Graphene
Christoph Schenke (Grenoble): Tonks-Girardeau Bosons Stirred on a 1D Ring

Mesoscopic Systems
Alfredo Levy-Yeyati (Madrid): Andreev Transport in Carbon Nanostructures
Juan-Carlos Cuevas (Madrid): Supercurrents in Microwave-Irradiated Superconducting Nanostructures
Moshe Goldstein (Yale): Quantum Impurity Model for Microwave Photons
Paco Guinea (Madrid): Closing Remarks

PCAM Summer School 2011: Electronic and Optical Properties of Nanoscale Materials

July 4-7, 2011

CHAIRMAN
Jose M. Pitarke (CIC nanoGUNE and UPV/EHU, Spain)

ORGANIZING COMMITTEE
Gian Paolo Brivio (U. Milano-Bicocca, Italy)
Ricardo Díez Muiño (CFM-CSIC and UPV/EHU, Spain)
Iñaki Juaristi (UPV/EHU)
Enrique Zarate, Secretary General (CIC nanoGUNE, Spain)

The PCAM (Physics and Chemistry of Advanced Materials) European network of doctorate programmes organizes every year a summer school on a specific relevant topic. The 2011 edition was organized by the University of the Basque Country (UPV/EHU), the Materials Physics Center CSIC-UPV/EHU, Donostia International Physics Center (DIPC), and the Nanoscience Cooperative Research Center nanoGUNE Consolider, in the framework of the Summer Courses of the University of the Basque Country. The lectures will focus on Electronic and Optical Properties of Nanoscale Materials. The participation is open to PhD students, post-docs, and all researchers interested in the field. The lecturers are first-class scientists and world leaders in their fields. The program, based on lectures and invited talks, also included oral contributions and a poster session.

Nanotechnology has set a new framework in material science where new materials are being designed for specific applications. A deep theoretical and experimental understanding is necessary to get insight and profit on the possibilities arising from the manipulation of materials at the nanoscale. The design of this course provides attendees with state-of-the-art knowledge on electronic and optical properties of nanoscale materials, most interesting in many applications such as nanodevices, sensoring, or medicine.

CONTRIBUTIONS

R. Martin (Illinois, USA)
Electronic structure of solids and nanoscale materials

J.J. Saenz (Madrid, Spain)
Photonic Materials

R. Berndt (Kiel, Germany)
Controlled single atom and single molecule contacts

C. Ocal (Barcelona, Spain)
Look closely at how and why supramolecular order influences

G. Drera (Milan, Italy)
A Resonant Photoemission Study Of LaAlO3-SrTiO3 Interface: Evidence Of In-gap Ti· + Electronic States

O. Idigoras (San Sebastian, Spain)
Anomalous Hard Axis Behavior In Uniaxial Co-films

E.J.G. Santos (San Sebastian, Spain)
Spin-Strain Phase Diagram Of Defective Graphene

J. Fransson (Uppsala, Sweden)
Theory For Spin-polarized STM Applied To Local Spins

R. Martin (Illinois, USA)
Electronic structure of solids and nanoscale materials

J.J. Saenz (Madrid, Spain)
Photonic Materials

A. Valsesia (Varese, Italy)
Nanoplasmonic devices, the next generation of ultrasensitive multiplexing biosensors

R. Hillenbrand (San Sebastian, Spain)
Infrared and Terahertz near-field nanoscopy

C. Motta (Milan, Italy)
Conducting Properties Of Diarylethene-based Molecular Switch On Graphene Leads

M. Gobbi (San Sebastian, Spain)
Magnetoresistance In Ferromagnetic-fullerene Hybrid Devices

P. Koval (San Sebastian, Spain)
O(N^3) Implementation Of Hedin's GW Approximation With Dominant Products Basis

B. Rousseau (San Sebastian, Spain)
Response Functions Through Wannier Interpolation

M. Chhowalla (New Jersey, USA)
Graphene

J. Kirschner (Halle, Germany)
Spin-Polarized STM and Nanomagnetism

S. Roche (Barcelona, Spain)
Exploring Quantum Transport in Graphene-based Devices: From Novel Device Principles to Spintronics

C. Gómez-Navarro (Madrid, Spain)
Chemically derived graphene: electronic and mechanical properties

M. Chhowalla (New Jersey, USA)
Graphene

J. Kirschner (Halle, Germany)
Spin-Polarized STM and Nanomagnetism

M.I. Trioni (Milan, Italy)
Theoretical treatment of electronic properties of single adsorbates on extended substrate

P.M. Echenique (San Sebastian, Spain)
Electron dynamics at surfces and nanostructures

L. Martin-Gondre (San Sebastian, Spain)
Energy Dissipation IN The Scattering Of Nitrogen off Ag(111) Surface

I. Goikoetxea (San Sebastian, Spain)
Non-adiabatic Effects During The Dissociative Adsorption Of O2 At Ag(111)?
A First principles Divide and Conquer Study

D. Gallach (Madrid, Spain)
Properties Of ZnO/Psi/Si Structures Prepared By The Sol-gel Technique

A. García-Lekue (San Sebastian, Spain)
Switching Of Molecular Conductivity Under Electric field

Workshop on Graphene

August 29–September 2, 2011

ORGANIZING COMMITTEE
Godfrey Gumbs
Yonatan Abraynos
Andres Ayuela
Francisco Guinea
Paula Fekete

CONTRIBUTIONS

Ricardo Díez-Muiño (Director of Centro de Física de Materiales, Spain)

Chairperson Professor Godfrey Gumbs (CUNY, USA)

Philip Kim (Columbia University, USA)
Manifest of electron interactions in quantum Hall effect in graphene

Klaus Zeigler (Universität Augsburg, Germany)
Collective modes of graphene

Shengjun Yuan (IMM, The Netherlands)
Modeling Electronic Properties of Single-layer and Multilayer Graphene

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Chairperson Dr. Danhong Huang (AFRL, USA)

Y.H. Chiu (NCKU, Taiwan)
Magneto-optical excitation of graphene under periodic magnetic field

Elton J.G. Santos (DIPC, Spain)
Magnetism of graphene with defect vacancies, substitutional metals and covalent functionalization

---

Chairperson Yonatan Abranyos (CUNY, USA)

Francesco Guinea (ICMM, Spain)
Electron-electron interaction in graphene

Charles Smith (University of Cambridge, United Kingdom)
Using low temperature scanning probe techniques to study graphene quantum dots

Yen-Hung Ho (NCKU, Taiwan)
The electronic and optical properties of graphene layers in response to magnetic field

Yurii Lozovik (MIPT, Russia)
Collective and coherent properties of graphene

Rafael Roldán (IMM, the Netherlands)
Bernstein modes in graphene

Luis Brey (ICMM, Spain)
Dirac electrons in superlattice potentials

Emmanuele Cappelluti (ICMM, Spain)
Spectral properties of phonon peaks in optical conductivity of graphene

Oleksiy Roslyak (CUNY, USA)
Charged particle energy loss in epitaxial, irradiated and free-standing multilayer graphene

W. Silkin (DIPC, Spain)
Unoccupied electronic states in layered graphene

Maria Vozmediano (ICMM, Spain)
General relativity and graphene

Leonid Levitov (MIT, USA)
States with spontaneously broken time reversal symmetry in graphene

---

Chairperson Paula Fekete (USMA, USA)

Wen Xu (ISSP, China)
Infrared optoelectronic properties of graphene and its application in HgCdTe infrared detectors

Mahi Singh (UWO, Canada)
Photon switching mechanism in graphene and quantum dot hybrid systems

Eugene Kogan (Bar-Ilan, Israel)
The influence of near-neighbor model in graphene on the dielectric function and plasmons

María P. López-Sancho (ICMM, Spain)
The effect of pressure on the magnetic moments of multilayer graphene

---

Chairperson Dr. Danhong Huang (AFRL, USA)

Fernando de Juan (IU, USA)
Aharonov-Bohm interferences from local deformations in graphene

Cristina Hernández Fuentevilla (USAL, Spain)
Transmission and conductance across a square barrier potential in monolayer graphene

---

Chairperson Mahi Singh (UWO, Canada)

Andres Ayuela Fernandez (DIPC, Spain)
Edge states and flat bands in graphene nanoribbons with arbitrary geometries

Enrique Diez (USAL, Spain)
Metal-insulator transitions in graphene

Hector Ochoa (ICMM, Spain)
Spin-orbit coupling and spin relaxation mechanisms in graphene

Paula Fekete (USMA, USA)
Effects of a potential barrier on spin currents along a nanotube

Amaia Zurutuza (Graphenea, Spain)
Graphenea and experiments at nanoGUNE

Mestizajes. Encuentro Internacional sobre Literatura y Ciencia

Mestizajes. Transitando las fronteras entre arte, ciencia y humanismo

Octubre 18-19, 2011

CHAIRMAN
Gustavo Ariel Schwartz (Centro de Física de Materiales/CSIC)

CO-CHAIRMAN
Juan Colmenero (DIPC, Jakiunde and CFM)

COMITÉ ACADÉMICO
Emmánuel Lizcano Fernández (UNED)
Ricardo Diez Muino (CFM - CSIC)
Silvina Cerveny (CFM - CSIC)
Andoni Ibarra (UPV/EHU)

¿Es posible un diálogo entre Ciencia y Literatura? ¿Tienen acaso algo que decirse?
¿Qué pueden aportarse mutuamente? ¿Es posible (y deseable) esta interacción?
¿O acaso ya existe sin que nos lo propongamos?

Mestizajes se propone como un espacio donde ponentes invitados debatirán con los asistentes estas (y otras) cuestiones mediante una serie de workshops y conferencias.

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 y conferencias 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.

Encuentro Internacional sobre Literatura y Ciencia
Los encuentros se llevarán a cabo en dos modalidades. Por las mañanas se realizará un Workshop en el Donostia International Physics Center (DIPC) donde los invitados disertarán acerca de diferentes aspectos sobre literatura y ciencia (ver temas del encuentro) y habrá un espacio para la discusión y el debate. Por la noche tendrán lugar las conferencias con ponencias individuales o mesas redondas sobre cada una de las áreas de interés del encuentro. Podrán encontrar información más detallada en las páginas del Worshop o de las Conferencias.

En esta ocasión, el tema de debate se centrará en la frontera entre Literatura y Ciencia. Nos proponemos explorar las formas de representación, la autorreferencialidad, los dualismos y el uso de modelos y metáforas tanto en ciencia como en literatura. Indagaremos sobre los distintos tipos de relaciones entre literatura y ciencia y exploraremos las posibilidades de ese espacio común situado en la frontera entre ambas.

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 se propone como un ámbito abierto y estimulante donde explorar ese territorio virgen, esa "terra incógnita", que se encuentra en la frontera entre ciencia y arte. Mestizajes pretende contribuir a la construcción de un conocimiento más amplio donde arte, ciencia y humanidades se complementen y se enriquezcan mutuamente.

Temas del encuentro
- Las formas de representación en literatura y en ciencia.
- La autorreferencialidad en ciencia y en literatura.
- Metáforas y modelos.
- El pensamiento contemporáneo.

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Posibles cuestiones para el debate
¿Cómo condicionan las formas de representación nuestra mirada sobre lo representado? ¿Puede el punto de vista cambiar nuestra interpretación acerca de lo que vemos? ¿Vemos o miramos? ¿Existe realmente una división clara entre objeto y sujeto? ¿Qué ocurre cuando el sujeto coincide con el objeto? ¿Qué problemas aparecen cuando la ciencia o la literatura indagan acerca de ellas mismas? El problema del otro. Limitaciones del pensamiento dualista. ¿Utiliza metáforas la ciencia? ¿Cuál es la diferencia entre metáforas y modelos? ¿Pueden las metáforas potenciar el conocimiento? Conocimiento holístico y conocimiento reduccionista. Ventajas y limitaciones de las categorías. Aspectos culturales de las formas de representación. ¿A qué responden los cambios de representación?

Workshop

Luisa Etxenike
En cuerpo y alma. Las formas de representación en Literatura y Ciencia

Alberto Rojo
Poesía y Física

Discusión/Mesa redonda: Luisa Etxenike y Alberto Rojo
Moderador: Gustavo Schwartz

Marta Macho-Stadler
Las matemáticas del OuLiPo

Gustavo Vargas Silva y Gorka Calzada Terrones
La experiencia de coescribir literatura científica infantil y juvenil.
Biografía de leonhard euler escrita a cuatro manos

Enkarni Gomez Genua y Ainhoa Güemes Moreno
(Im)Precisiones para una Gnoseología Artecnocientífica Artecnociencia y Feminismos

Guillermo Roa
Microciencia: Ciencia a través del micro
Moderadora: Luisa Etxenike

Guillermo Martínez
Autorreferencia en Literatura y Matemática

Luis Sáez Rueda
La 'Mathesis Universalis' como patología de Occidente y los cauces emergentes para su rebasamiento.

Mesa redonda

Guillermo Martínez / Luis Sáez Rueda
Moderador: Andoni Ibarra

Agustín Fernández Mallo
El mundo como diseño: las ciencias como representación.
Moderadora: Silvina Cerveny
Cierre: Gustavo Schwartz

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Conferencias

Luisa Etxenike/Alberto Rojo
En cuerpo y alma. Las formas de representación en Literatura y Ciencia. Poesía y Física
Moderador – Gustavo Schwartz

Bernardo Atxaga
Reacciones ante una piedra rayada
Moderador: Juan Colmenero

Guillermo Martínez / Luis Sáez Rueda
Autorreferencia en Literatura y Matemática.
La 'Mathesis Universalis' como patología de Occidente y los cauces emergentes para su rebasamiento
Moderador: Andoni Ibarra

Mariasun Landa Etxebeste / Agustín Fernández Mallo
Espacios entre las fronteras de la ciencia y la literatura.
El mundo como diseño: las ciencias como representación
Moderadora: Silvina Cerveny

Network Meeting of the European project "CUBiHOLE", ERANET project

October 26-29, 2011

ORGANIZER
Javier Aizpurua

This Network meeting was devoted to analizee the progress on the European project CUBiHOLE, an ERANET project prioritized by the European Union, and funded by the Spanish Ministry within the program of Internationalization. The aim of this project is to build, characterize optically and understand clusters of metallic nanoparticles linked by organic cages (cucurbiturils) as hybrid platforms to host optoelectronic processes and devices.The first part of the Workshop took place in Hondarribia, where a set of technical talks devoted to report on the progress of each aspect of the project was developed. The Chemical group from the university of Cambridge reported on the last progress on CBs synthesis, the group from the University of Bordeaux reported on the recent achievements on electrochemical synthesis of hybrid systems, the Optical group of the University of Cambridge reported on the optical characterization of the clusters by measuring optical extinction, and SERS activity on the metallo-organic platform. The group from DIPC reported on the latest advances in the theoretical characterization of the physics of aggregation of the particle clusters, and on the processes involving tunneling between the particles.

The second part of the workshop took place at Donostia International Physics Center in Donostia, where a full day of the Meeting was devoted to analyze the perspectives and potential of the project CUBiHOLE from the point of view of intellectual property (IT). To that end, a group of experts in IT from Cambridge University Enterprise, an Agency of the University of Cambridge dealing with intellectual property issues managed a full session to identify the main topics and potentials of the project on the short, medium and long term for commercial explotation.

2011

http://dipc.ehu.es

Credits
Creative direction and design: Lauren Hammond (iGn) <laurenhammond@gmail.com>
Text coodination and editing: Marimar Alvarez <m-alvarez@ehu.es>
Photography: Alex Iturralde (www.alexiturralde.com)
Printing: Reproducciones Igara (www.igara.com)

http://dipc.ehu.es

Paseo Manuel de Lardizabal, 4 ▪ E-20018 Donostia-San Sebastián