
Donostia International Physics Center
PASSION FOR
KNOWLEDGE
Celebrating 10 years
Activity Report
08/09

On the cover

Steps of silicon serve as a natural ruler for measuring vertical dimensions. This silicon "target" has step heights ranging from tens to hundreds of nanometers leading down to a flat, single atomic layer measuring only 0.3 nanometer. The microscope used to make this image sits on an isolated concrete slab equipped with air springs to cancel out even minute vibrations that could ruin the nanoscale measurements.

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DIPC Activity Report 08/09

Committed to the public diffusion of science

Pedro Miguel Echenique, President of DIPC, starts the session for Encounter with Nobel Laureates in kutxaEspacio de la Ciencia, part of the Atom by Atom program

Celebrating 10 years of DIPC

In 2010, DIPC celebrates its tenth anniversary, and although this report accounts for the last biannual period, it is appropriate for us to look back at our beginnings and reflect on the covered path after a decade.

DIPC was established on the grounds and buildings of a former school property of the city of Donostia-San Sebastian, adjacent to the university campus. The site was ideally placed, facing the Faculty of Chemistry of the University of the Basque Country, arguably the most prestigious research center in the country.

For years, we had reflected on the type of institution that was needed to promote science in the Basque Country, and envisaged it as an adaptable agent capable strengthening areas where our existing players needed support. They in turn, would not find in DIPC another counterpart, but a partner who facilitates their growth and international projection. Bringing this innovative and unconventional project to fruition represented a challenge to us, as promoters, as well as to prospective partners and authorities responsible for backing our undertaking. The project was to materialize into four seminal programs: DIPC was to act as a hub of internationalization, bringing prestigious foreign researchers into contact with our own investigators for periods that sealed new professional links. In addition, it would act as a landing platform for brilliant Basque postdoctoral scientists after their training abroad. Thirdly, the center would house seminars, workshops and courses in which the above interacted with students and researchers from our institutions. Finally, we were committed to working on the public diffusion of science, and aspired to bring science and scientists closer to society.

In order to fulfill all these goals, we counted with university and CSIC staff acting as the core of the organization. A contingent of temporary young members (Fellows Gipuzkoa) would be associated to the institution for up to five years. Finally, visiting senior scientists for periods up to one year would not only bring invaluable talent and experience, to all the other contingents, but would become our acting ambassadors abroad.

Juan Colmenero
Director

Celebration of a shared success

Alberto López
Secretary

Our project received an outstanding reception from our public institutions. The city transferred the school grounds to the foundation, and the Basque Government supported the refurbishment of the buildings, the installation of scientific equipment and a state of the art computer facility. Generous support from the Provincial Authority of Gipuzkoa provided us with precious start-up resources, the Fellows Gipuzkoa program, and moral backing. The University of the Basque Country, with whom we shared our objectives, became and continues to be our solid academic partner. We were privileged to count with the participation of our private patrons: kutxa, Iberdrola, Naturgas Energía, Telefónica, CAF, and Mapfre. Their step forward firmly completed an exemplary public-private partnership of strategic breadth.

I vividly remember all those who first contributed to our launching ten years ago. They have since become permanent members of our community and dear friends to this day. On completion of its first year, DIPC had already received 24 visitors, housed 17 seminars and organized 4 workshops, counting with no less than 54 international publications. Thereafter, our family kept growing year after year.

On its tenth anniversary year, the center's indicators reached a record 163 international publications, 46 seminars and 8 workshops. We received 184 visitors, of which almost a third remained with us for periods longer than 6 months. After a decade of activity, our collaborators have participated in 1192 scientific articles in internationally acclaimed journals.

The outreach activity of DIPC over the last decade combined regular lectures for the general public with major events directed at communicating the values and enthusiasm for science around a theme. In September 2005, coinciding with the centenary of Albert Einstein's annus mirabilis, we organized a three-day public celebration of science, attended by no less than 1,400 members of the public who enjoyed the inspiring presentations of exceptional scientists. At the time, we were surprised and delighted to witness the enthusiasm manifested by members of the public as well as our speakers. In 2009, DIPC participated in the organization and backing of a second public conference, on occasion of the official launching of the associated nanoscience and nanotechnology center CIC nanoGune. The event, entitled Atom by Atom was also massively attended, receiving much public acclaim. Coverage of Atom by Atom can be found on the following pages.

PASSION FOR KNOWLEDGE
Celebrating **10 years**

Finally, and as a landmark of our tenth anniversary, we are launching the Passion for Knowledge conference in September 2010. On this occasion, the celebrated topic will be the quest for knowledge itself, as seen through the eyes of extraordinary speakers from a wide range of disciplines.

My final words of this message are dedicated to my close associates, DIPC director Juan Colmenero and secretary Alberto López, as well as our administrative and technical staff. Finally, our heartfelt gratitude to the patrons of the foundation who shared our vision and aims, participated in our endeavor, and contributed the necessary resources. Many thanks to the Basque Government Departments of Industry and Education, the Provincial Authority of Gipuzkoa, through the Department of Innovations and Knowledge Society and the city of Donostia-San Sebastian, for their admirable support. I also wish to express my deep gratitude to our current private patrons, kutxa, Naturgas Energía, Telefónica, CAF, and Mapfre for their inspiring involvement and backing of the project. And finally, this project largely owes its success to the endeavor and support of the University of the Basque Country. The human capital and resources offered by the university have been incalculable throughout this decade.

After ten years of activity the DIPC project has been refined and consolidated as a model for the empowerment of established academic and research institutions, and we continue to develop the center with new initiatives and refreshed enthusiasm. This biannual Activity Report is both evidence and celebration of a shared success.

Pedro Miguel Echenique

Message from the President

Our Patrons

Basque Government
José Antonio Campos Granados (2008)
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Minister of Education, Universities and Research

Ana Aguirre Zurutuza (2008)
Bernabé Unda Barturen (2009)
Minister of Industry, Innovation, Commerce and Tourism

Ibone Amezaga Arregui (2008)
Pedro Luis Arias Ergueta (2009)
Deputy Minister of Universities and Research

José Ignacio Tellechea Fernández (2008)
Pedro Hernández González (2009)
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Joaquín Villa Martínez Adviser to the Statutory Deputy, Innovation and the Society of Knowledge

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Odón Elorza González Mayor
María Soledad Garmendia Beloqui (2009) Town councillor for Innovation and Presidency

kutxa
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Naturgas Energía
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Cesar Alierta Izual President

Construcciones y Auxiliar de Ferrocarriles
Andrés Arizkorreta García General Director

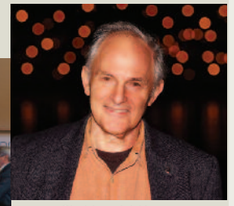
MAPFRE S.A.
Filomeno Mira Candel Vice President

Pedro Miguel Echenique and Albert Fert

Cristina Uriarte, María Isabel Celaá, Pedro Miguel Echenique, Patxi López, José María Pitarke, Marisol Garmendia, and Rafaela Romero

José María Pitarke and Igor Campillo

Pedro Miguel Echenique, María Isabel Celaá, and Heinrich Rohrer



Sir Harold Kroto

Sir John Pendry

Carlos Ruiz

Atom by Atom... into nanoscience

The Atom by Atom conference co-organized by DIPC and nanoGUNE between September 28th and 30th, 2009, took the audacious step of bringing together beneath a single umbrella an international scientific conference (NANO2009) and a series of activities focusing on bridging the gap between science and the general public. At DIPC, we feel responsible to the international scientific community and to our citizens for conveying knowledge and contributing to progress, culture and freedom in society. Our aim is to provide meeting places for scientists and between science and society. We'd like to think that we achieved just that with Atom by Atom and must say that we're proud of our efforts.

Atom by Atom was opened to the general public via its plenary section for the purpose of bringing together scientific rigor and entertainment to foster an immersion in science as a cultural activity. The Atom by Atom plenary section, involving an outstanding line-up of speakers featuring three Nobel laureates and renowned researchers, presented a program of conferences and activities open to the public addressing an extensive range of topics in which nanotechnology is expected to have a powerful impact, such as electronics, health or new materials.

Atom by Atom was a success because it had extraordinary speakers, because it was an opportunity to share our projects with them, because the standard of contributions received and because the standard of the plenary lectures was extremely high. But, above all, Atom by Atom was a success thanks to the extent of citizen response to our call.

Monday, September 28	**812** participants
Tuesday, September 29	**948** participants
Wednesday, September 30	**615** participants

Public attendance well overshot our expectations as we saw how the talks and activities were followed with tremendous interest and enthusiasm. That's why we at DIPC and nanoGUNE are even more determined to continue concentrating on our undertaking of bringing science to society.

ATOMBYATOM
into nanoscience

Welcome

Pedro Miguel Echenique (left),
Patxi López Álvarez (center),
President of the Basque Government,
and **José María Pitarke** (right)

Opening Lecture

Sir Harold Kroto
1996 NOBEL PRIZE IN CHEMISTRY

Science, society and sustainability

Performance

Pep Bou

Rebufaplanetes

Encounter with Nobel Laureates
in kutxaEspacio de la Ciencia

Nobel Laureates **Heinrich Rohrer** (left) and **Sir Harold Kroto** (right) participated in an interactive session for school children. The session was moderated by **Pedro Miguel Echenique** (center).

Felix Goñi
UPV/EHU, Biophysics Unit, Centro Mixto CSIC-UPV/EHU (Spain)
Lipidic nanoparticles: fat is beautiful

Emilio Mendez
Brookhaven National Laboratory (USA)
Nanotechnology and the energy challenge

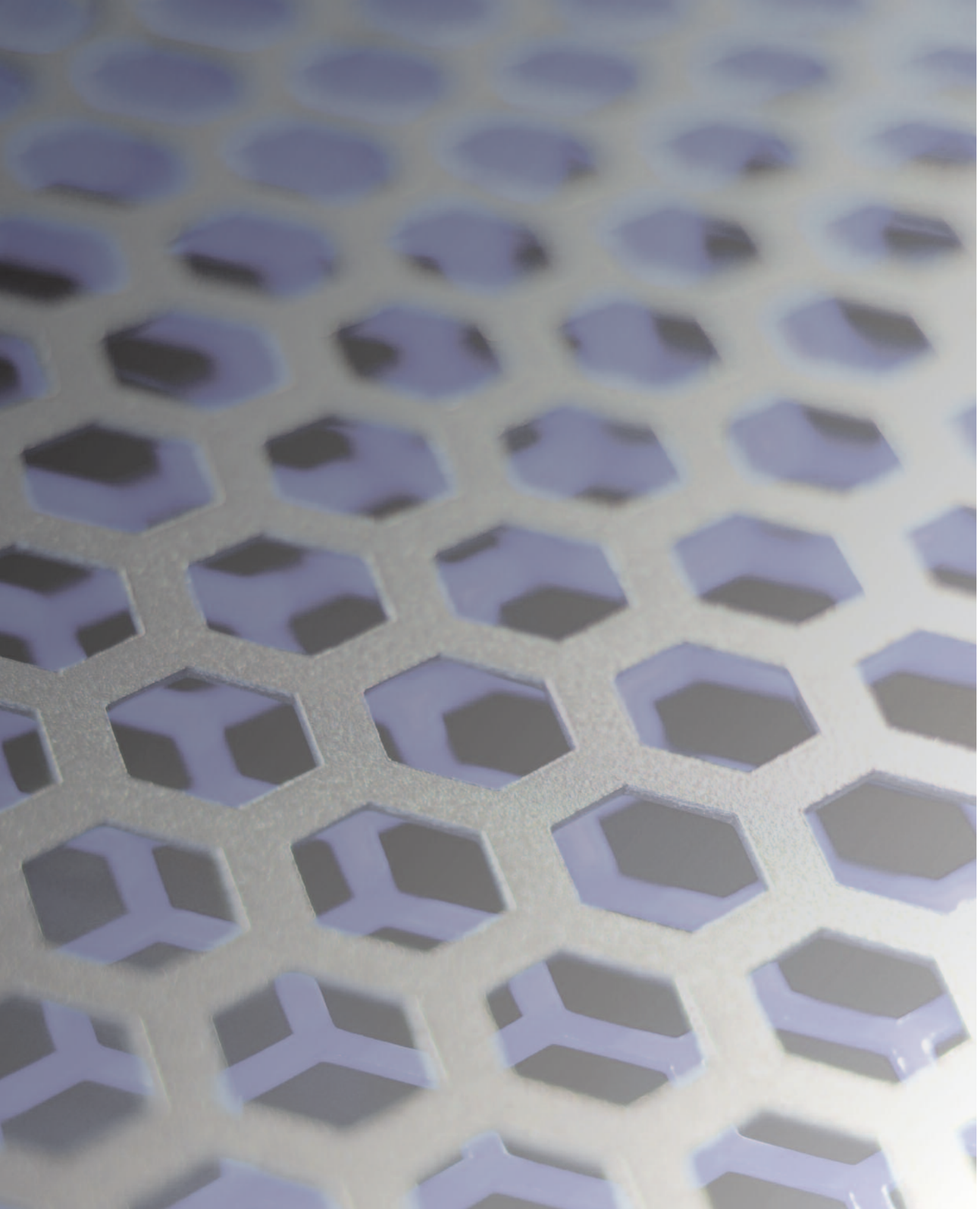
Carlos Bustamante
University of California, Berkeley (USA)
Grabbing the cat by the tail: DNA packaging motor

Juan Colmenero
UPV/EHU, CSIC-UPV/EHU, DIPC (Spain)
Molecule by molecule:
Molecular self-assembly and nanotechnology

Jose Maiz
Intel Corporation (USA)
Nanoscience and nanotechnology:
The promise, the reality, and the challenges

Sir John Pendry
Imperial College London (UK)
Transformation optics and nanotechnology

Albert Fert
2007 NOBEL PRIZE IN PHYSICS
Université Paris-Sud, Unité Mixte de Physique CNRS/Thales (France)
Spintronics: fundamentals, recent developments and perspective



Research Activity

1192 scientific articles

18,000 quotations
(Approximation as of April 2010)

2000-2009

1228 visiting researchers

432 seminars

51 conferences

5083 participants

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

Scientific Highlights

Index

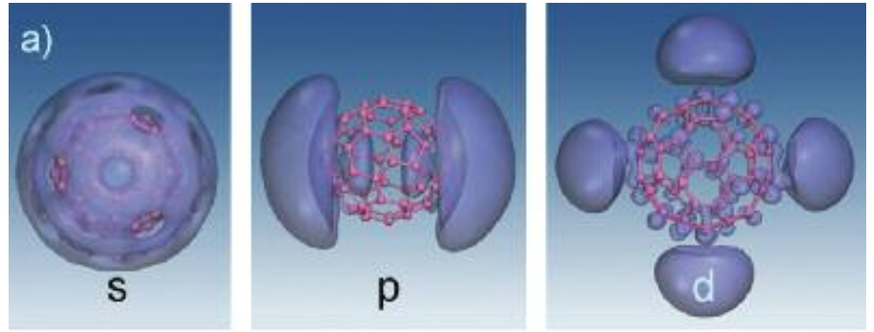
Molecules behaving like atoms

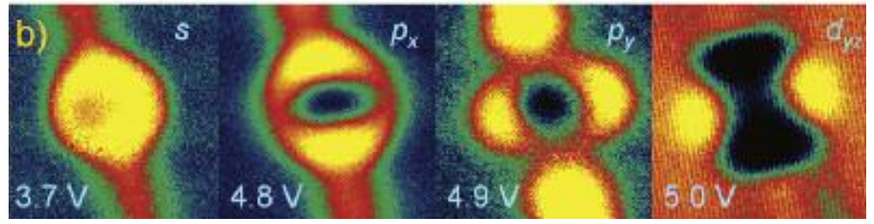
M. Feng, J. Zhao, and H. Petek
Science 320, 359 (2008)

A team from the University of Pittsburgh and Donostia International Physics Center discovered atom like molecular orbitals of hollow molecules. In a scanning tunneling microscopy (STM) study of C_{60} molecule, a hollow cage of sixty carbon atoms in the shape of a soccer ball, they found images suggesting that under some circumstances hollow molecules can exhibit electronic properties that mimic atoms. When several such molecules are combined into linear chains or close-packed islands, electrons injected into atom-like molecular orbitals delocalize as they would in a metal.

The characteristic properties of conductivity and reflectivity arise from the propensity of metal atoms to give up their electrons. If organic molecules could learn the same trick, they could become versatile components of molecule-based electronics. The team found that hollow molecules, such as C_{60}, behave as superatoms: at certain bias voltages they bind added electrons not to individual atoms, like other molecules, but to their empty core, giving them appearance of large atoms in STM images. When two hollow molecules come together, their images resemble those of diatomic molecules. For larger one- or two-dimensional aggregates the images resemble free-electron alkali metals. The atom-like properties of C_{60} molecules are reproduced by density functional theory calculations.

The theoretical modeling suggests that the origin of superatom states are the image potential states of a two-dimensional carbon sheet, graphene. Such image potential states were discovered and have been studied for metals and liquid He in the pioneering theoretical work of Pendry and Echenique. The superatom states are derived form the image potential states of graphene through a topological distortion into a sphere. The discovery of superatom states in C_{60} molecules provides the first experimental and theoretical verification of image potential states of molecular sheets. The attribution of superatom states to the universal origin in the image potential states of a molecular sheet suggests that hollow molecules of other materials should exhibit similar properties, and it suggests new strategies for design of novel molecular electronic materials.





a) The theoretical and b) experimental images of the superatom orbitals of C_{60} molecule. The theoretical images indicate the existence of unoccupied orbitals of C_{60} and other hollow molecules with spatial distributions of *s*, *p*, *d*, ... symmetry spherical harmonic orbitals of atoms, corresponding to orbital angular momentum l=0, 1, 2.... Molecular orbitals with distinctly atom-like s, p, and d character have been discovered through spectroscopic imaging in a low temperature STM.

The discovery of superatom states in C_{60} molecules provides the first experimental and theoretical verification of image potential states of molecular sheets.

High-level correlated approach to the jellium surface energy, without uniform-electron-gas input

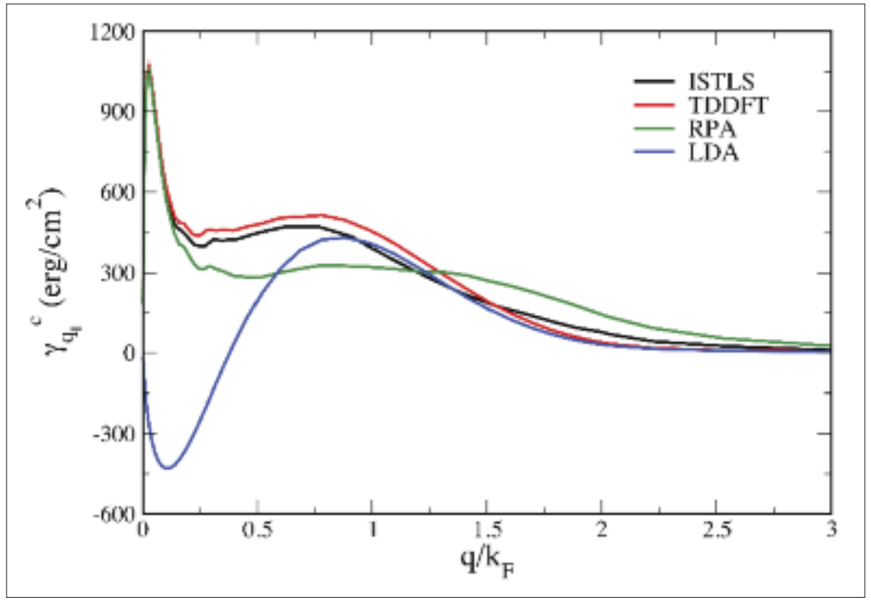
L.A. Constantin, J.M. Pitarke, J.F. Dobson, A. Garcia-Lekue, and J.P. Perdew
Physical Review Letters 100, 116102 (2008)

We resolve the long-standing controversy over the metal surface energy: Density-functional methods that require uniform-electron-gas input agree with each other, but not with high-level correlated calculations such as Fermi-hypernetted-chain and diffusion-Monte-Carlo calculations that predict the uniform-gas correlation energy accurately. Here we apply the inhomogeneous Singwi-Tosi-Land-Sjölander method, and find that the density functionals are indeed reliable. Our work also vindicates the use of uniform-gas-based nonlocal kernels in time-dependent density-functional theory.

Density-functional theory (DFT) provides ground-state electron densities and energies [and, in its time-dependent version (TDDFT), excitation energies] for atoms, molecules, and solids. Because of its simple self-consistent-field structure, DFT is used for electronic-structure calculations almost exclusively in condensed matter physics, and heavily in quantum chemistry. Exact in principle, the theory requires in practice approximations for the exchange-correlation (xc) energy (and the socalled xc kernel of TDDFT) as a functional of the density. All commonly used nonempirical approximations require input from the uniform electron gas, which is transferred to inhomogeneous densities. The reliability of these approximations must be judged a posteriori, and there had been for many years a long-standing puzzle related to their reliability for solid surface energies, with implications for vacancies and clusters. The surface energy is not only of technological importance, but also a classic and highly sensitive test case for theories of exchange and correlation in manyelectron systems.

Here we develop a very high-level correlated many-body approach that generalizes the well-known orbital-based Singwi-Tosi-Land-Sjölander (STLS) formalism to the case of inhomogeneous systems, and we resolve the long-standing controversy over the reliability of existing densityfunctional calculations of metal surfaces energies. Our calculations lead us to the conclusion that the existing DFT calculations are reliable (in contrast with the then available high-level correlated Fermi-hypernetted-chain and diffusion-Monte-Carlo calculations). An analysis of the surface energy into contributions from dynamical density fluctuations of various two-dimensional (2D) wave vectors is also reported, which rules out the belief that the local-density approximation for the particle-hole interaction (in the context of TDDFT) might be inadequate for the description of the surface energy of simple metals.

We resolve the long-standing surface-energy controversy.



2D wave-vector analysis of the correlation surface energy of a jellium slab of thickness 7.21 r_s (r_s = 2.07). Black, red, green, and blue lines represent inhomogeneous-STLS (ISTLS), uniform-gasbased TDDFT, random-phase-approximation (RPA), and local-density-approximation (LDA) calculations, respectively. q is the magnitude of the 2D wave vector (in the surface plane) of the density fluctuations. The area under each curve amounts to the correlation surface energy in units of erg/cm^2. k_F represents the magnitude of the Fermi wave vector. r_S represents (in units of the Bohr radius) the radius of a sphere that encloses one electron on average. We observe that in the longwavelenght limit (small q) both ISTLS and TDDFT calculations coincide with the RPA, which is exact in this limit, while the LDA fails badly. In the large-q limit, both ISTLS and TDDFT calculations approach the LDA, as expected, while the RPA is wrong. Two independent schemes (the ISTLS approach, which does not use and isotropic xc kernel derived from the uniform gas, and the TDDFT approach, which uses a uniform-gas-based isotropic xc kernel) yield essentially the same wave-vector analysis of the correlation surface energy. This supports the conclusion that the local-density approximation for the particle-hole interaction is indeed adequate to describe simple metal surfaces.

Our work vindicates the use of uniform-gas-based nonlocal kernels in time-dependent density-functional theory.

Role of electron-hole pair excitations in the dissociative adsorption of diatomic molecules on metal surfaces

J.I. Juaristi, M. Alducin, R. Díez Muiño, H.F. Busnengo, and A. Salin
Physical Review Letters 100, 116102 (2008)

The role of electronic excitations in the dissociation of molecules at metal surfaces has been studied. The validity of the Born Oppenheimer approximation to describe this kind of processes has been proven.

The Born-Oppenheimer approximation is the usual starting point in the theoretical study of the interaction of thermal molecules with surfaces. Among other things, this approximation involves to neglect the energy loss suffered by the molecule along its trajectory as a consequence of the electronic excitations that it induces in the metal. Paradoxically, the experimental evidence of these excitations is such that their existence is out of question. The great controversy in this field is related to the question of which is the real importance of electronic excitations to determine the dissociation of the molecules or, more generally, the reactivity of the molecules at surfaces. With the aim of gaining knowledge on this question, a theoretical model has been developed, totally based on *ab initio* calculations, which also incorporates the electronic excitations into the dynamic equations. The contribution of electron-hole pair excitations to the reactive dynamics of H_2 on Cu(110) and N_2 on W(110) has been evaluated, including the six dimensionality of the process in the entire calculation. The interaction energy between molecule and surface is represented by an *ab initio* six-dimensional potential energy surface. Electron friction coefficients are calculated with density functional theory in a local density approximation. The two systems that have been considered represent two cases in which the dissociation dynamics is completely different. In H_2/Cu(110), the dissociation is ruled by a late activation barrier, at short distances from the surface. It is at these distances where the molecule finds high electron densities and where larger energy losses are more likely to occur. On the other hand, in N_2/W(110), the dynamics is more involved and combines direct and trapping mediated dissociation mechanisms. The dissociation of N_2 on metal surfaces has been considered as an emblematic example of a system where electronic friction can be relevant. The reasoning behind that assumption was the high value of the friction coefficient for N atoms moving in electronic media.

The results of our calculations showed that the contribution of electron excitations is a marginal correction to the dissociation dynamics and, therefore, that an adiabatic calculation is still meaningful for a wide range of situations. It was also shown that the low velocity of the reacting molecules in the surface regions of high electronic density is the main reason to explain this fact. This leads us to conclude that the theoretical models based on the Born-Oppenheimer approximation capture the main physics of the adsorption dynamics for these systems.

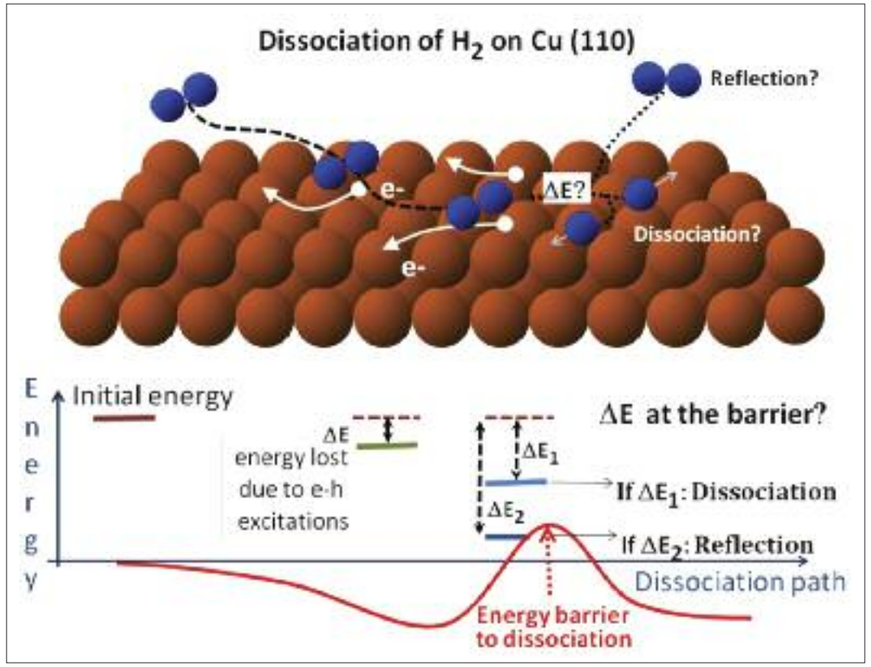


Figure 1. Schematic representation of the energetics of the interaction and the dynamics of H_2 at Cu(110).

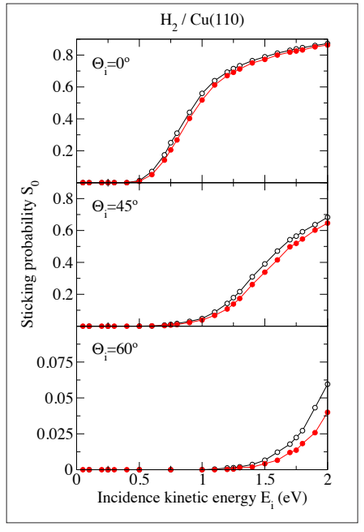


Figure 2. Dissociative sticking probability for H_2/Cu(110) at different incident angles. Full red (open black) circles are the results with (without) electronic friction.

We calculate for the first time the contribution of the electronic excitations to the dissociation of diatomic molecules at metal surfaces keeping the six dimensionality of the problem in the whole calculation.

Formation of dispersive hybrid bands at an organic-metal interface

N. Gonzalez-Lakunza, I. Fernández-Torrente, K.J. Franke, N. Lorente, A. Arnau, J.I. Pascual
Physical Review Letters 100, 156805 (2008)

A combined STS and DFT study of the interface between the monolayer of donor-acceptor TTF-TCNQ complex and a Au(111) substrate reveal that organic-metal dispersing hybrid bands, that have both metal and molecular character, are formed at the interface as a result of a complex mixing between molecular orbitals, mainly through TTF, and metal states. These results suggest that, by tuning the components of such molecular layers, the dimensionality and dispersion of organic-metal interface states can be engineered.

The use of organic thin films in electronic devices requires the existence of electronic bands with high conduction properties, but, organic materials inherently have narrow bands and low electron mobility due to their weak intermolecular interactions. Organic-inorganic hybrid materials have been proposed as the ideal framework to merge the high carrier mobility of metals with the advantageous properties of organic materials. However, this approach remains sustained in empirical bases. A molecular scale conceptual picture of the cross talk between organic and metallic states in the formation of organic-metal (OM) hybrid bands is still missing.

Scanning tunneling microscope (STM) experiments, carried in ultrahigh vacuum and low temperature, show that TTF and TCNQ deposited on Au(111) self-assemble into mixed domains of alternating rows of donor and acceptor species with a 1:1 stoichiometry. In contrast to the TTF-TCNQ molecular solid bulk phase where molecules are π-stacked, here they lie parallel to the surface, as we can determine from their intramolecular structure [Fig. 1a)]. Such adsorption structure is confirmed by first principles calculations. The relaxed geometry of the TTF-TCNQ layer on Au(111) [Fig. 1b)-c)] shows that the molecular layer is bonded to the gold substrate trough the TTF. However, the most interesting properties of this OM system are revealed by scanning tunneling spectroscopy (STS) measurements.

In this work [1], we show that OM hybrid bands are formed at the interface between the donor-acceptor TTF-TCNQ complex and the Au(111) substrate. The bands combine a reduced dimensionality imprinted by the overlayer structure with a large dispersion reminiscent of its metallic character. By means of a combined STS and density functional theory (DFT) study [Fig. 2], we find that the bands originate from a complex mixing of metal and molecular states. While the TCNQ is essentially unperturbed by the underlaying surface, the TTF is hybridized with the Au(111) surface. The result is the formation of two interface bands with both molecular and metal character. They exhibit a free-electron metal-like dispersion and the anisotropic structure of the molecular layer.

This study allows us to obtain a conceptual understanding about the formation of OM hybrid bands. Our results suggest that tuning the strength of donor-metal interaction or spacing between the TTF rows may allow one to engineer the organic-inorganic interface band structure and, hence, the functionality of the molecular thin film.

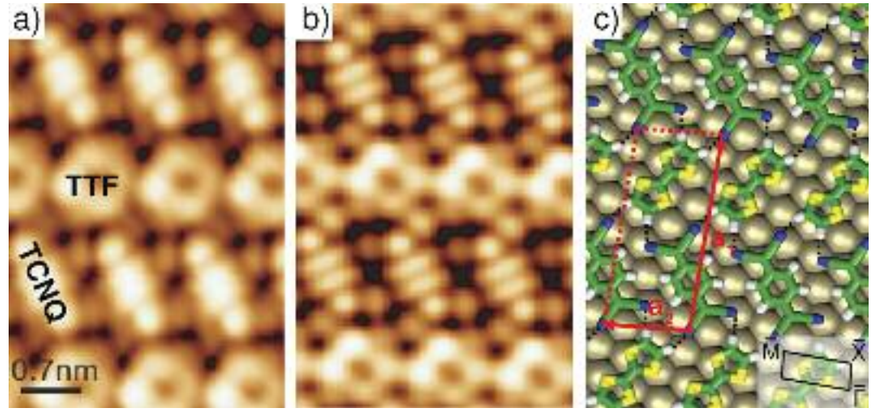


Figure 1. a) STM image with intramolecular resolution of the TTF-TCNQ mixed domain (V = 0.3 V; I = 0.4 nA). The molecular structure of TTF and TCNQ resembles the shape of the respective HOMO and LUMO. b) Simulated constant current STM image (V = 1.0 V) using the Tersoff-Hamman approach on the DFT optimzed geometry shown in c). c) The vectors a1 and a2 define the commensurate surface unit cell and the inset correspond to the SBZ.

An electronic band with quasi 1D dispersion is found at the metal-organic interface.

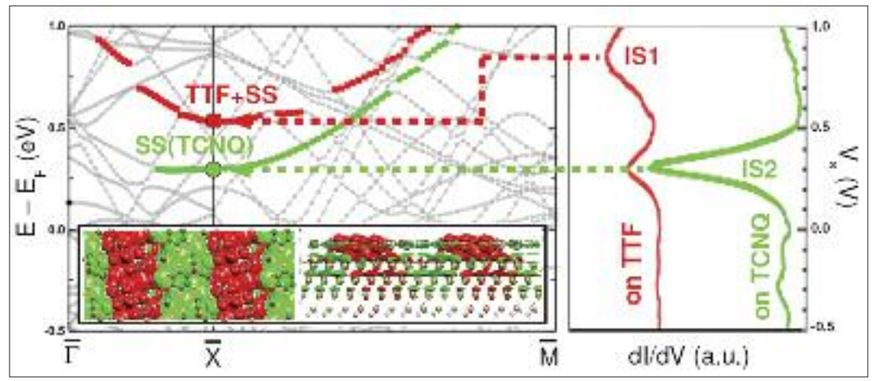


Figure 2. At the left part, the calculated band structure of TTF-TCNQ on Au(111) is shown, where the states that have some interface character has been coloured. Two bands can be distinguished: in green, a band that disperses along the molecular rows, and that has mainly metal character as it can be seen in the spatial charge distribution at Γ shown in the inset; and in red, a band with a bi-dimensional dispersion, mix of TTF and Au. At the right part, the experimental STS spectra taken onto TTF, in red, and onto TCNQ, in green, show two distinct features, IS1 and IS2, that are associated to the two calculated interface bands.

Resonant plasmonic and vibrational coupling in a tailored nanoantenna for infrared detection

F. Neubrech, A. Pucci, T. W. Cornelius, S. Karim, A. Garcia-Etxarri, and J. Aizpurua
Physical Review Letters 101, 157403 (2008)

A novel resonant mechanism involving the interference of a broadband plasmon with the narrow-band vibration from molecules is presented. With the use of this concept, the authors demonstrate experimentally the enormous enhancement of the vibrational signals from less than one attomol of molecules on individual gold nanowires, tailored to act as plasmonic nanoantennas in the infrared.

Vibrational spectroscopy of molecules is of general importance in natural sciences, medicine, and technology. Direct infrared (IR) observation of molecular vibrations from a reduced number of molecules is a current challenge in all these fields. The respective sensitivity can be increased by several orders of magnitude with the use of surface-enhanced scattering techniques such as surface-enhanced Raman scattering (SERS) and surface-enhanced IR absorption (SEIRA).

In this study, the authors make use of IR antennas to boost the sensitivity of a SEIRA experiment. An IR antenna is a metallic nanostructure that acts as an effective receiver and transmitter of infrared light. It has the ability to confine the incident electromagnetic radiation to tiny spots of nanometer-scale dimensions (hot spots). This nanoscale concentration of the light permits to sense a much smaller amount of molecules than a regular SEIRA experiment.

This work shows both theoretical and experimentally that the effect of the resonant coupling of an individual plasmonic IR nanoantenna with the vibrational excitation of small number of molecules produces a different type of resonant SEIRA with unprecedented signal enhancement of 5 orders of magnitude, which means attomol sensitivity. The enhancing effect occurs only when the resonant interaction between both excitations (antenna and molecular vibration) is achieved, as proven by calculations.

To achieve a completely resonant situation, the length L of the nanoantenna is designed to hold a plasmonic resonance exactly matching the spectral position of the vibrational fingerprints of the molecules. Because of the finite negative value of the dielectric response of gold in the IR, antenna resonances in the μm range of the spectrum appear for slightly shorter L than the ideal half-wave dipole antenna length. With help of exact EM calculations, carried out by the nanophotonics group of the DIPC, that correctly predict the spectral resonance position of such a system, the authors are able to engineer the geometrical characteristics of the nano-antenna to obtain the resonance at the required IR wave- length and measure the vibrational signal of the molecules with unprecedent sensitivity.

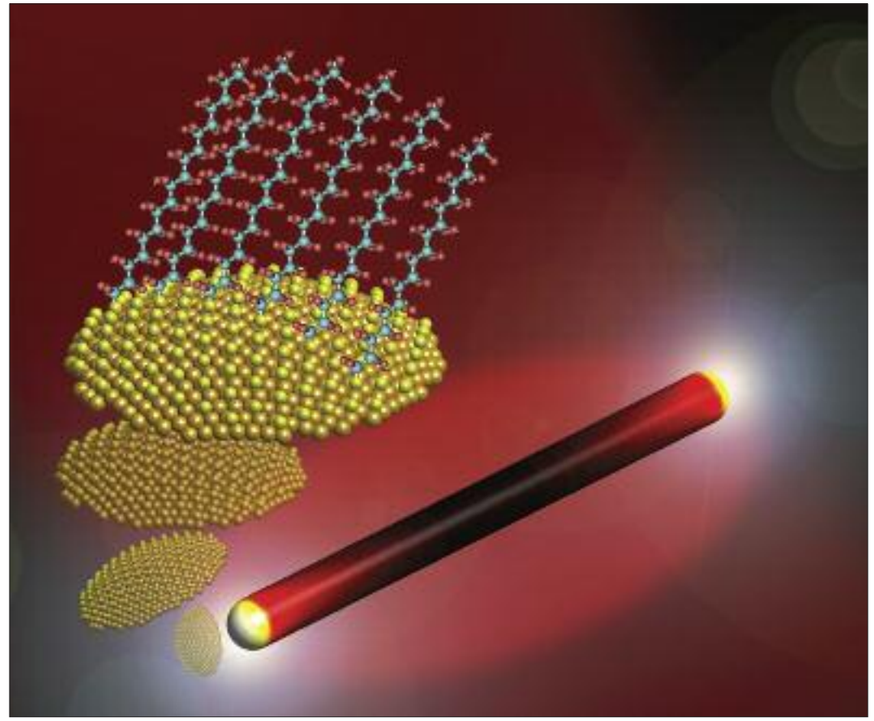
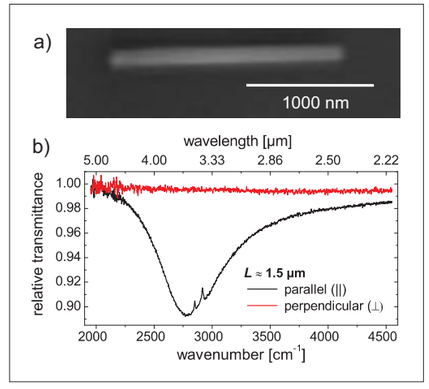


Figure 1. Sketch showing the experimental setup. A monolayer of octadecanthiol (ODT) molecules is deposited on a single IR resonant antenna. The system is illuminated with light polarized parallel to the antenna axis, and the transmittance of the system is measured.



Few thousand molecules detected employing an IR nanoantenna as a near-field enhancing mechanism.

Figure 2. a) Scanning electron micrograph of a gold NW with similar dimensions as used in this study.
b) Relative IR transmittance in the spectral region of the fundamental resonance of a gold NW with one ODT monolayer for parallel (||) and perpendicular polarization (⊥). A CaF2 substrate is used. The broadband plasmonic resonance is observed around λ≈3.6μm.

Complex quasiparticle structure induced by electron-phonon interaction: band splitting in the 1x1H/W(110) surface

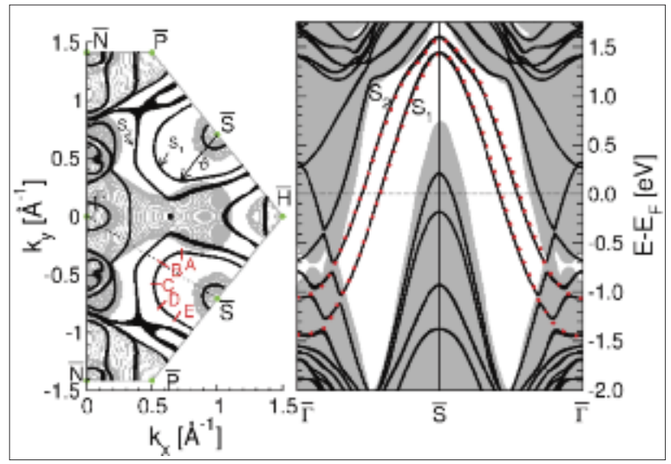
Asier Eiguren and Claudia Ambrosch Draxl
Physical Review Letters 101, 036402 (2008)

We show that the self-consistent solution of the complex Dyson equation for the electron-phonon (EP) problem introduces many body effects which are often observed in photoemission experiments. The formalism is applied to the H covered W(110) surface, using first-principles results for the electronic and vibrational structure. We demonstrate that the measured spin-polarized surface band splitting [Phys. Rev. Lett. 84, 2925 (2000); 89, 216802 (2002)] can be traced back to different quasiparticle (QP) states induced by EP coupling. Despite the breakdown of the single QP picture, the spectral functions are very well represented by the predicted multiple QP structure.

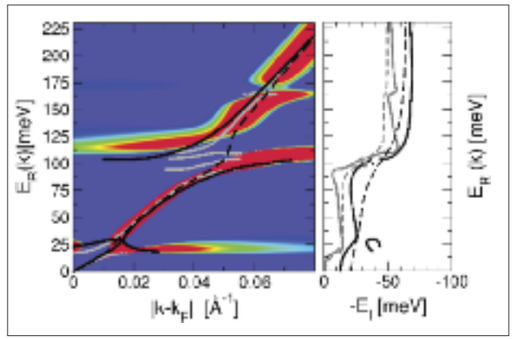
Recent developments in angle-resolved photoemission spectroscopy (ARPES), revealing subtle details of the electronic structure, pose a challenge for a proper theoretical interpretation. Many 2D systems exhibit peculiarities in the measured spectral functions which are far from the ideal Lorentzian shape. Such observations include materials as different as bulk graphite and high-Tc cuprates and one clear possible origin can be found in electron-phonon (EP) coupling. This interaction is usually more pronounced in low dimensions, one prominent example being the hydrogen covered W(110) surface. In this system, for one of the surface states, experiment indicates the occurrence of two clear structures in the ARPES spectra, both with well defined energy dispersion [1]. Thereby, isotope substitution provided striking evidence for EP interaction being the source for the band splitting. The fact that the surface states are spin polarized as well as spin-orbit (SO) split, adds more interesting features to this already puzzling situation. We have included the spin-orbit interaction in the unperturbed electron structure calculation.

In this work we show that electron-phonon interaction indeed leads to multiple quasiparticle (QP) states. The key point is that the electron self-energy is not only a complex function, but also a complex function of complex (energy) argument. Indeed, we show that the analytic continuation to complex energies is not trivial. In this way, a complex Dyson equation can be defined for complex quasiparticle poles, which can be considered as self-consistently renormalized. Technically, our method is an important extension of Engelsberg and Schrieffer work [Phys. Rev. 131, 993], to finite temperatures and for generic Eliashberg functions.

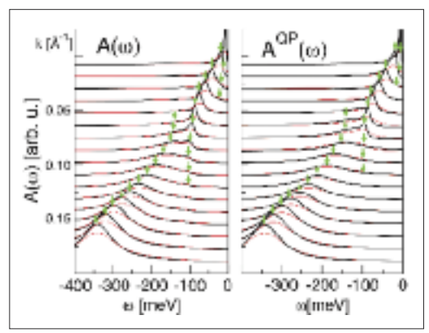
An application to the 1x1H/W(110) surface demonstrates that several experimentally observed quasiparticle states are present in the calculation, offering an explanation detected many-body band splitting in photoemission measurements.



Left: Fermi surface of the slab system. Right: electron bands along $\bar{\Gamma}\,\bar{S}$, the grey area indicating the projected bulk bands. Red dots highlight the S_1 and S_2 bands.



Self-consistent solution of the complex Dyson equation for H/W(110). Left: QP bands (solid lines) at T=150K (black) and 40K (grey). The background color presents the second derivative of the spectral function at T=40K. Right: inverse lifetimes $1/\tau = |\,E_I\,|$ (solid) and bare self-energies $1/\tau^0 = |\,\Sigma_I\,|$ (dashed) at T= 40K (grey) and T=150K (black).



Spectral functions, A_k (ω), at T=40K (thick black) and T=150K (thin red) of H/W(110) for different momenta compared to their counterparts in the multiple quasiparticle approximation, $A_k^{QP}(E) \equiv \sum_n \mathrm{Im}\left[\frac{-Z^{qp}(k,n)/\pi}{E - E^{qp}(k,n)}\right]$.

Entangledlike chain dynamics in nonentangled polymer blends with large dynamic asymmetry

A. J. Moreno and J. Colmenero
Physical Review Letters 100, 126001 (2008)

Simulations of a nonentangled polymer blend with large dynamic asymmetry reveal novel features for chain relaxation of the confined fast component. The latter strongly resemble usual observations for entangled homopolymers. We suggest a more general frame, beyond reptation models, for dynamic features usually associated to entanglement effects.

We have performed molecular dynamics simulations on a simple model for polymer blends (Figure 1). The selected values for the chain length N are in all cases much smaller than the entanglement length of the corresponding homopolymer. A large dynamic asymmetry between the two components in the blend induces strong confinement effects for the fast component. At odds with standard predictions of the Rouse model, strong nonexponential behaviour for the Rouse normal modes is observed for the confined fast component. From simple scaling arguments we infer that strong nonexponentiality is an intrinsic feature which does not arise from a simple distribution of elementary exponential processes. Despite simulated chains being much shorter than the entanglement length, strong dynamic asymmetry induces dynamic features, as anomalous scaling properties for the Rouse modes (see Figure 2), resembling observations in strongly entangled homopolymers. Very recent simulations of chemically realistic blends [Brodeck et al., Macromolecules, to be published] confirm this observation, suggesting that this is a general feature of polymer blends with large dynamic asymmetry.

This unusual behaviour is associated to strong memory effects which break the Rouse-like assumption of time uncorrelation of the external forces acting on the tagged chain. The observed anomalous scaling laws for the Rouse modes strongly resemble predictions from recent theoretical approaches based on generalized Langevin equations (GLE). Within the approach of renormalized Rouse models for the memory kernel, nonexponentiality and anomalous scaling are directly connected to slow relaxation of density fluctuations around the tagged chain. The latter may be induced by entanglement, but data reported here for the fast component suggest that this is not a necessary ingredient. Analogies with entangledlike dynamics are indeed observed even for N = 4 monomers, provided that dynamic asymmetry in the blend is sufficiently strong.

The results of this work suggest a more general frame, beyond usual reptation-based models, for chain relaxation features usually associated to entanglement effects. They also open new possibilities for the application of GLE methods in complex polymer mixtures.

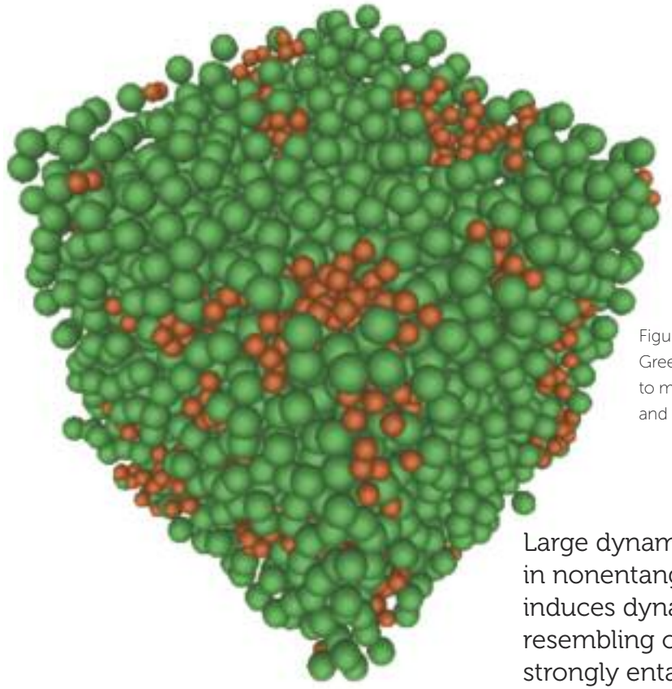


Figure 1. Snapshot of a simulation cell. Green and orange spheres correspond to monomers of, respectively, the slow and fast components of the blend.

Large dynamic asymmetry in nonentangled polymer blends induces dynamic features resembling observations in strongly entangled homopolymers.

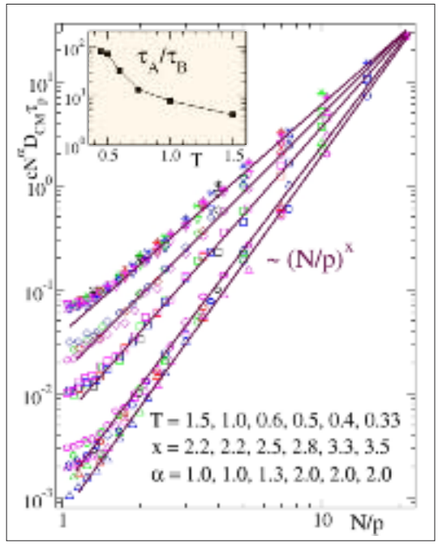


Figure 2. Main panel: For the fast B-component in the AB-blend, scaling of the relaxation times of the chain normal modes, τ_p, versus their wavelength N/p. Inset: Temperature (T) dependence for the ratio of the structural relaxation times of the slow A- and fast- B components, which quantifies dynamic asymmetry. N is the number of monomers per chain. D_{CM} is the diffusivity of the chain center-of-mass. Each symbol code corresponds to a different temperature (see legend), and each color code to a different N. Lines describe power law behavior ~ $(N/p)^x$. The exponent changes from standard Rouse behavior, x ≈ 2, at high T (weak dynamic asymmetry) to anomalous behavior, x ≈ 3.5, at low T (strong asymmetry).

We suggest a more general frame, beyond reptation-based models, for chain relaxation features usually associated to entanglement effects.

Dynamic arrest in polymer melts: competition between packing and intramolecular barriers

Marco Bernabei, Angel J. Moreno and Juan Colmenero
Physical Review Letters 101, 255701 (2008)

By means of simulations, we investigate the role of intramolecular barriers on the glass transition of polymers. An analysis within the framework of the Mode Coupling Theory reveals a fundamental difference between the nature of the glass transition in polymers and in simple glass-formers.

Since they do not easily crystallize, polymers are probably the most extensively studied systems in relation with the glass transition phenomenon. Having said this, their macromolecular character, and in particular chain connectivity, must not be forgotten. Another particular ingredient of polymers is the presence of intramolecular barriers. Thus, they are responsible of partial or total crystallization, and can enhance reptation effects. Semiflexible polymer models are of great interest, since they can be applied to many important biopolymers. Thus, an understandig of the structural, dynamical and rheological properties of semiflexible polymers is of fundamental as well as of practical interest. In this work we present computer simulations of a simple bead-spring model for polymer melts with intramolecular barriers, covering the range from fully-flexible to stiff chains (Figure 1). By systematically tuning the strength of the barriers, we investigate their role on the glass transition. Dynamic observables are analyzed within the framework of the Mode Coupling Theory (MCT) of the glass transition. Critical nonergodicity parameters, critical temperatures and dynamic exponents are obtained from consistent fits of simulation data to MCT asymptotic laws.

The so-obtained MCT λ-exponent increases from standard values, characteristic of simple glass-formers, for fully-flexible chains, to values close to the upper limit λ = 1 for stiff chains (see Figure 2). In analogy with systems exhibiting higher-order MCT transitions, we suggest that the observed large λ–values arise from the interplay between two distinct mechanisms for dynamic arrest: general packing effects and polymer-specific intramolecular barriers. With this, the systematic study of the effect of intramolecular barriers presented here establishes a fundamental difference between the nature of the glass transition in polymers and in simple glass-formers.

The study presented here establishes a fundamental difference between the nature of the glass transition in polymers and in simple glass-formers.

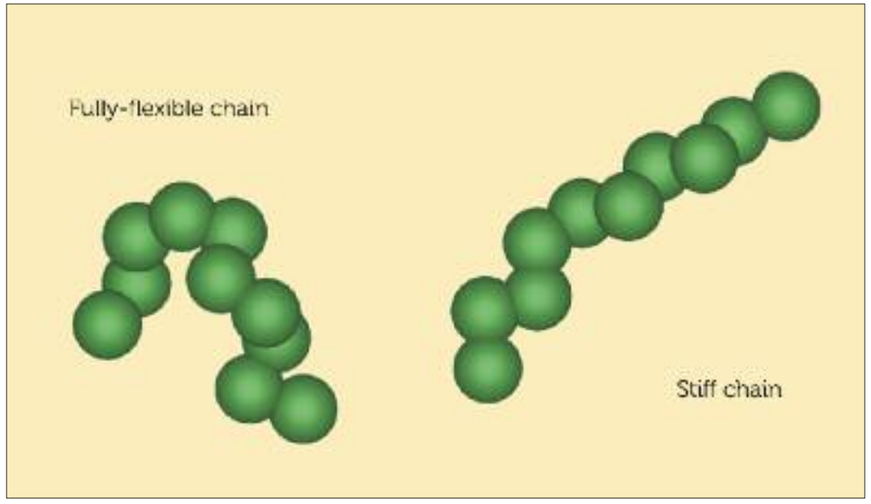


Figure 1. Typical conformations of fully-flexible and stiff simulated chains.

A higher-order MCT scenario arises from the interplay between two distinct mechanisms for dynamic arrest: general packing effects and polymer-specific intramolecular barriers.

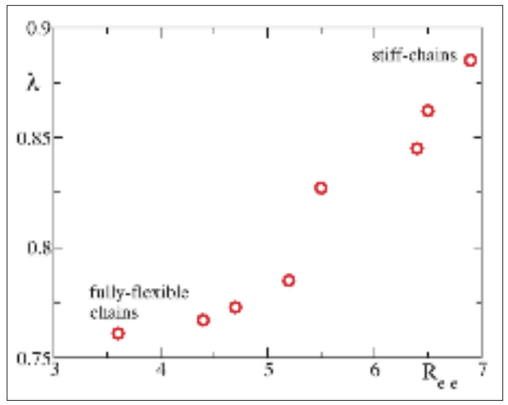


Figure 2. Variation of the MCT λ-exponent with the average chain end-to-end radius, which quantifies chain stiffness.

Controlling the near-field oscillations of loaded plasmonic nanoantennas

M. Schnell, A. Garcia-Etxarri, A. J. Huber, K. Crozier, J. Aizpurua and R. Hillenbrand
Nature Photon 3, 287-291 (2009)

An innovative method for controlling light on the nanoscale by adopting tuning concepts from radio-frequency technology is presented. The method opens the door for targeted design of antenna-based applications including highly sensitive biosensors and extremely fast photo-detectors for biomedical diagnostics and information processing.

An antenna is a device designed to transmit or receive electromagnetic waves. Radio frequency antennas find wide use in systems such as radio and television broadcasting, point-to-point radio communication, wireless LAN, radar, and space exploration. In turn, an optical antenna is a device which acts as an effective receiver and transmitter of visible or infrared light. It has the ability to concentrate (focus) light to tiny spots of nanometer-scale dimensions, which is several orders of magnitude smaller than what conventional lenses can achieve. Tiny objects such as molecules or semiconductors that are placed into these so-called "hot spots" of the antenna can efficiently interact with light. Therefore optical antennas boost single molecule spectroscopy or signal-to-noise in detector applications.

In this study, the researchers studied a special type of infrared antennas, featuring a very narrow gap at the center. These so called gap-antennas generate a very intense "hot spot" inside the gap, allowing for highly efficient nano-focusing of light. To study how the presence of matter inside the gap (the "load") affects the antenna behavior, the researchers fabricated small metal bridges inside the gap (Figure b). They mapped the near-field oscillations of the different antennas with a modified version of the scattering-type near-field microscope that the Max Planck and nanoGUNE researchers had pioneered over the last decade. For this work, they chose dielectric tips and operated in transmission mode, allowing for imaging local antenna fields in details as small as 50 nm without disturbing the antenna. By monitoring the near-field oscillations of the different antennas with this novel near-field microscope, it is possible to directly visualize how matter inside the gap affects the antenna response. The effect could find interesting applications for tuning of optical antennas.

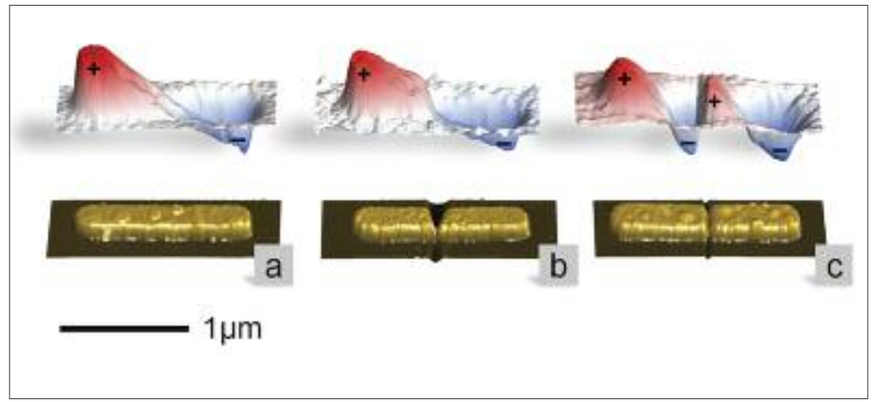
Bridging the gap in nanoantennas.

The nanooptics group from DIPC fully confirmed and helped to understand the experimental results by means of full electrodynamic calculations. The calculated maps of the antenna fields are in good agreement with the experimentally observed images. The simulations add deep insights into the dependence of the antenna modes on the bridging, thus confirming the validity and robustness of the "loading" concept to manipulate and control nanoscale local fields in optics.

Furthermore, the researchers applied the well developed radio–frequency antenna design concepts to visible and infrared frequencies, and explained the behavior of the loaded antennas within the framework of optical circuit theory. A simple circuit model showed remarkable agreement with the results of the numerical calculations of the optical resonances. By extending circuit theory to visible and infrared frequencies, the design of novel photonic devices and detectors will become more efficient. This bridges the gap between these two disciplines.

With this work, the researches provide first experimental evidence that the local antenna fields can be controlled by gap-loading. This opens the door for designing near-field patterns in the nanoscale by load manipulation, without the need to change antenna length, which could be highly valuable for the development of compact and integrated nanophotonic devices.

Nanoantenna loading allows for near-field control in the nanoscale.



Near-field microscope images of loaded infrared antennas. The bottom line depicts the topography, whereas the upper line plots the scanned near-field images. Figure a) shows a metal nanorod that can be considered the most simple dipole antenna. The near-field image clearly shows the dipolar oscillation mode with positive fields in red and negative fields in blue color. By introducing a narrow gap at the center of the nanorod thus altering the "antenna load" (Figure c), two dipolar-like modes are obtained. When the gap is connected with a small metal bridge (Figure b), the dipole oscillation mode of Figure a) can be restored as the near-field image clearly reveals.

Novel structures and superconductivity of silane under pressure

Miguel Martinez-Canales, Artem R. Oganov, Yanming Ma, Yan Yan,
Andriy Lyakhov, and Aitor Bergara
Physical Review Letters 102, 087005-8 (2009)

Understanding the complex behavior of the simplest element remains a hot topic in condensed matter physics. Soon after the BCS theory for superconductivity was established, Neil W. Ashcroft realized that a very high Tc was plausible. Nevertheless, 70 years after metallic hydrogen was predicted, it still is an elusive goal of physics. Main arguments leading to a high Tc superconducting hydrogen are its light mass and the expected strong electron-ion interactions. It has been recently suggested that these arguments should also hold for metallic alloys with a high hydrogen content. The heavier elements in these alloys are expected to *"chemical precompress"* the hydrogen and, therefore, lower the pressure threshold required for the metallization. Group IVa hydrides have been pointed as obvious candidates. Between them, silane has been subject of most theoretical and experimental research so far, which has prompted us to thoroughly analyze compressed silane using *ab initio* methods coupled with evolutionary structure prediction algorithms.

According to our calculations (Figure 1), in the lower pressure range, between 10 and 25 GPa, the most stable structure is the molecular *P21/c*. At 25 GPa we have a pressure-induced structural transition to a phase of symmetry *Fdd*2. From the electronic point of view, the band gap has a drastic reduction and in the *Fdd*2 structure the gap decreases from 2 eV to 1 eV in its pressure range of stability. The presence of such small gap explains the strong changes in the optical properties: silane becomes completely black and opaque in this pressure range.

As seen in Figure 1, at 55 GPa there are four competitive structures (*Fdd*2, *I*41/*amd*, *P*2/*c* and *I*41/*a*) with the same enthalpy. The latter three structures share the presence of Si-H-Si chains and are radically different from the semimolecular *Fdd*2 (Figure 2). Actually, above 55 GPa the *Fdd*2 structure undergoes a significant change, as the second neighbors of H atoms are no longer H but Si and, therefore, increasing the pressure will not just compress the structure but favors the formation of polymeric Si-H-Si chains and makes unavoidable the transition to the also insulating *I*41/*a* phase, which remains stable up to 220 GPa.

In the high pressure range (Figure 1), insulating tetragonal *I*41/*a* eventually gives way to a new metallic structure of symmetry *Pbcn* (Figure 2), marking the threshold at which, according to our calculations, silane adopts a metallic ground state. The *Pbcn* structure shows an interlayer alloy-like atomic arrangement, with slightly displaced almost square Si layers and H atoms lying in the interlayer spaces of the structure. Given the layered character of the *Pbcn* structure and the high concentration of H atoms, it is likely that this structure might display electronic similarities to pure metallic hydrogen not seen in previously proposed structures. Interestingly, we have performed electron-phonon calculations at 190 GPa and according to the Allen-Dynes approximation, metallic *Pbcn* silane would become a superconductor with a *Tc* of 16.5 K.

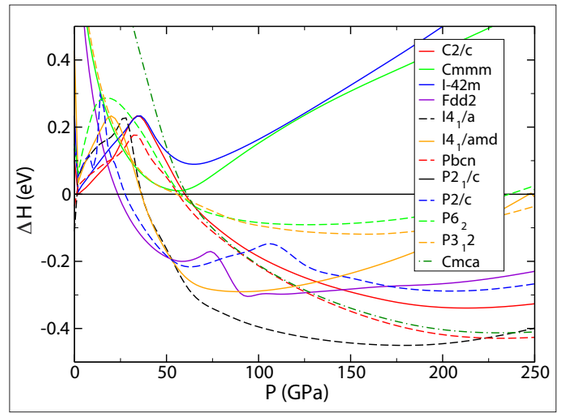


Figure 1. Enthalpies of the most favorable structures. Interestingly, at 55 GPa four competing structures have the same enthalpy and silane changes from intermediate between molecular and polymeric to a fully polymeric phase. The experimentally suggested $P6_3$ structure lies always at least 1 eV above the reference *P*21/*c* structure.

Heavier elements in hydrogen rich alloys chemically precompress hydrogen and lower the threshold pressure required for the metallization.

According to our calculations, silane might become a good superconductor above 200 GPa.

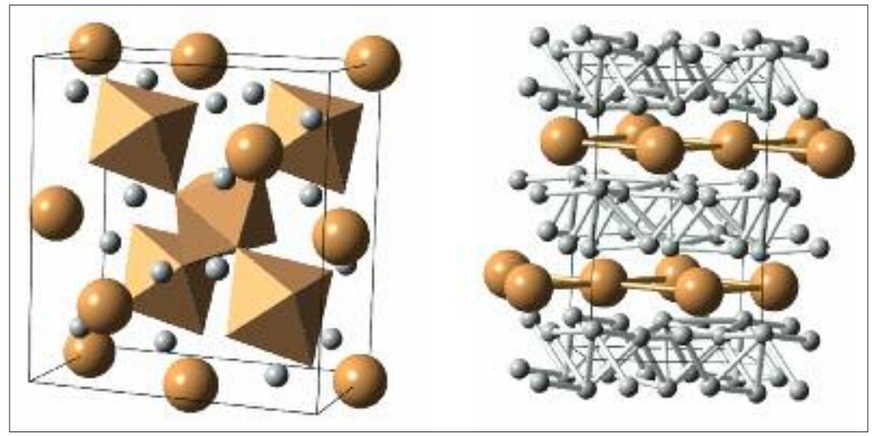


Figure 2. Novel structures of silane. Large atoms depict Si, while small atoms represent H. Left: *Fdd*2 silane, stable between 25 and 55 GPa. Right: *Pbcn* silane, which is metallic, superconducting and favored above 220 GPa.

Reduction of the superconducting gap in ultrathin Pb islands

Christophe Brun, I-Po Hong, François Patthey, I. Yu. Sklyadneva,
R. Heid, P.M. Echenique, K.P. Bohnen, E.V. Chulkov, and Wolf-Dieter Schneider
Physical Review Letters 102, 207002 (2009)

The fundamental question of how the superconducting properties of a material are modified when its thickness is reduced down to a few atomic monolayersis of special relevance for possible technological applications in superconducting nanodevices. The early model of Blatt and Thompson predicted an increase of the critical temperature T_c above the bulk value with decreasing film thickness, together with T_c oscillations due to quantum size effects. However, if proper boundary conditions allowing for spill-out of the electronic wave functions in thin films are taken into account, a decreasing T_c with decreasing film thickness was predicted. In this Letter, we report in situ layer-dependent STS measurements of the energy gap of ultrahigh-vacuum grown single-crystal Pb/Si(111)-7x7 and Pb-(√3x√3/)Si(111) islands in the thickness range of 5 to 60 monolayers (ML). Also employing layer-dependent \emph{ab initio} density functional calculations for free-standing Pb films, we find for thin layers a similar behavior of T_c, caused by a thickness dependent decrease of the electron-phonon coupling.

Figure 1 shows an STM image of a flat-top Pb island extending over two Si terraces separated by a single Si(111) step. The island mainly consists of an 8 ML thick Pb area with respect to the Si surface, as determined from the apparent height in the STM topograph. The island thickness includes the ≈1ML wetting layer. The inset shows a magnified view of the Pb surface lattice with atomic resolution.

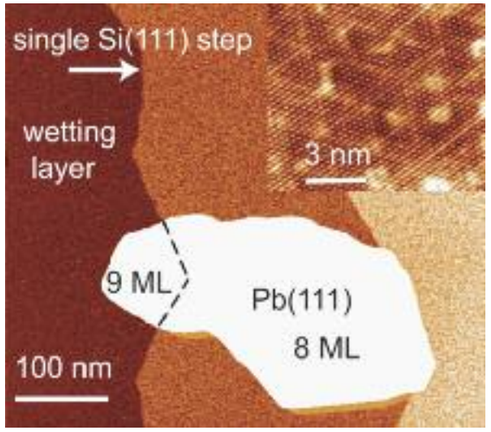


Figure 1. STM image of a flat-top Pb(111) single-crystal island grown on Si(111)-7x7. The island extends over two Si terraces. Island thickness includes the wetting layer. V_{bias} = -1.0 V, I = 100 pA. The inset shows a magnified view, revealing the Pb lattice with atomic resolution (V_{bias} = 20 mV, I = 1 nA).

For all thicknesses studied, the largest contribution to the e-ph coupling originates from electronic states of p_z symmetry: both surface- and bulk-like p_z states contribute to **λ**. The states of in-plain symmetry, p_x and p_y, play a minor role in the e-ph coupling. The e-ph coupling matrix elements do not affect qualitatively the phonon DOS F(**ω**): the calculated Eliashberg function **α**2F(**ω**) shows the same peak structure as the phonon DOS F(**ω**), all phonon modes contribute to **λ**. This result is in good agreement with the absence of significant changes in the measured phonon energies in the dI/dV spectra upon thickness reduction. Fig. 2 shows that the theoretical T_c are in fairly good agreement with the trend observed from the present STS data. The calculated T_c for the 5, 6 and 7 ML film are larger than those estimated from the measured gap values. This might be ascribed to the larger discrepancy arising at small film thickness between calculated and measured QWS energies, the latter being smaller.

For thin Pb islands on Si(111) the experimentally observed reduction of the superconducting energy gap with decreasing film thickness is consistent with the first principle results of a thickness-dependent e-ph coupling constant **λ**, where close to the ultrathin Pb film limit the variations of the density of states at E_F play a decisive role. Interestingly, both atomically smooth (Pb/Pb-√3x√3/Si) and disordered (Pb/Si-7x7) interfaces yield similar experimental behavior, in agreement with results showing that both systems are in the diffusive limit.

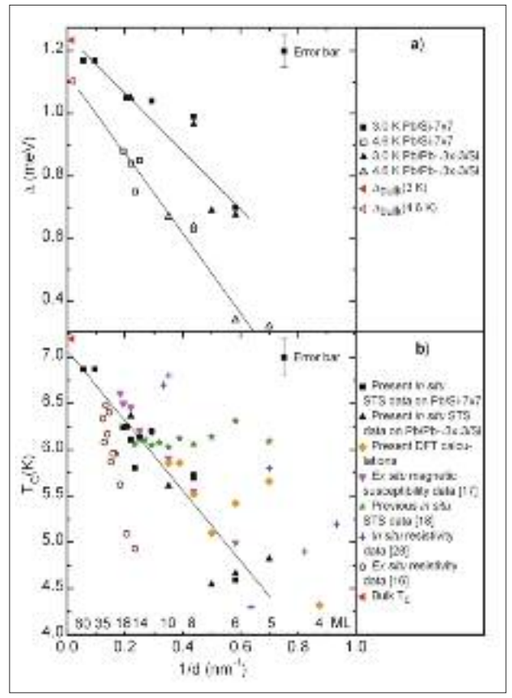


Figure 2. Superconducting energy gap Δ as a function of inverse Pb island thickness 1/d, extracted from BCS fits of dI/dV tunneling spectra, for the crystalline (Pb/Pb-√3x√3/Si) and disordered (Pb/Si-7x7) interface. Continuous lines are guide for the eyes. b) Estimated critical temperature T_c as a function of 1/d, using the bulk Δ/T_c ratio and assuming BCS temperature dependence of Δ(T), to allow comparison with previously reported results. Continuous line is a fit to the present STS data. For both a) and b) error bars: experimental dispersion and uncertainty in the fit results. All the references indicated can be found in the present publication reference list.

One-electron model for the electronic response of metal surfaces to sub-femtosecond photoexcitation

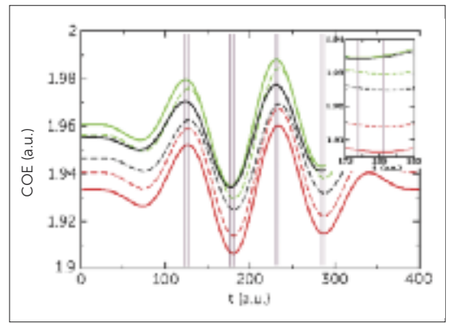
A.K. Kazansky and P.M. Echenique
Physical Review Letters 102, 177401 (2009)

One-dimensional model for analysis of sub-femtosecond streaking experiment with metal surface is suggested. The important features of the system, such as a pseudopotential for electron motion in the metal bulk, an abrupt decrease of the normal to the surface external electromagnetic field in the bulk, a finite value of the mean free path for electrons in the metal, and an action on the ejected electron of the (stationary) screened positive hole in the metal are included in the model. The results obtained in our computations reveal a simple dependence of the delay on the final energy of an electron ejected from the localized state. The results of our computations are in very good agreement with the measurements.

Study of the real-time dynamics of electrons in condensed-matter systems is pertinent for progress in nanotechnology. The electron processes in nano-systems are very fast and their investigation in real time requires application of experimental tools with sub-femtosecond time resolution. Recently, the first experiment [1] with streaking observation of electron dynamics in metal in the sub-femtosecond range was performed. In this experiment, the surface of solid was illuminated by two pulses. The first pulse was a short XUV pulse with the frequency of about 90 eV and duration (FWHM for the field envelope) of about 0.2 fs. Intensity of this pulse was quite low. Another pulse was a relatively strong (power W in 10^9 – 10^10 W/cm^2 range) near-infrared (NIR) laser pulse with the frequency of about 1.5 eV and with the duration of about 10 fs. The energy spectra of the electrons ejected from the localized f-state and delocalized band through the (110) surface of tungsten in the direction normal to this surface were measured. The time delay between the two pulses was varied and the energy spectra of the ejected electrons were monitored as a function of this delay. These energy spectra are the result of steering of the electrons, ejected from the metal by the XUV pulse, by the electric field of the NIR pulse in vacuum. The energy acquired by the ejected electron from the NIR field depends on the time of the electron passage across the metal surface. Thus, with measuring the dependence of the ejected electron energy spectrum on the time delay between the pulses, one can keep track on the process dynamics in the time domain.

The processes triggered by the instantaneous excitation of an electron in a solid are very complicated and a number of various mechanisms can be of paramount importance. First, electrons in the metal are moving in the field of the lattice. This can change the group velocity of the excited electron packet inside the bulk. Second, a localized electron after its ejection leaves in the bulk a positively charged hole which is then screened by the itinerant electrons. Third, the ejected electrons suffer inelastic collisions with electrons of the metal. This determines the depth from which the ejected electrons can reach the surface without inelastic collisions and thus carry direct information on the processes in the bulk. Fourth, the normal component of the laser field decreases in the bulk abruptly to a very small value under the condition of the experiment. This determines the peculiarity of streaking effect in the system considered.

We have formulated a simple and versatile model which allows one to estimate the magnitude of the possible effects and to analyze the influence of the parameters of the system on the output. Our model includes the main ingredients of the short time physics involved in the experiment. Within our model, we have computed the time-delay in the streaking spectra of the electrons ejected from the localized and localized electrons that was measured experimentally. The calculations, despite using a one-dimensional model potential, apply a time-dependent approach and take into account all relevant effects leading to a reasonable agreement with experiment. As a result of our computation, we have obtained for the time delay 85 attoseconds, while the experimental result [1] was at that time rather indefinite: 110±70 as. Later the experiment was repeated and the improved result is very close to our prediction. Worthy to emphasize that this is a unique result of a quantitative measurement of an phenomenon in a solid state with an attosecond experimental setup.



The positions of the center of energy of electron spectra ejected perpendicularly to the W surface are plotted. Solid lines correspond to the result for the total spectra, the red line shows the center of energy for electrons emitted from the delocalized initial state with the final energy E = 2 a.u., the black line corresponds to the same quantity obtained for the case of localized initial state with the final energy E = 2 a.u., and the green line gives the result obtained for the case of the initial local state, but with final energy E = 3 a.u. (The curves are shifted along the energy axis to the same scale.) The dashed lines, black and green, show contributions from the topmost atoms for the two values of final energy given above, and the dashed red line shows the center of energy for the electron ejected from the top of the delocalized band. The computed energy shift is clearly seen in the insert as a difference in position of minima of the curves.

We determine the peculiarity of streaking effect in the system considered.

Hydrogen-bonding fingerprints in electronic states of two-dimensional supramolecular assemblies

N. Gonzalez-Lakunza, M.E. Cañas-Ventura, P. Ruffieux, R. Rieger, K. Müllen, R. Fasel, A. Arnau
ChemPhysChem, 10, 2943-2946 (2009)

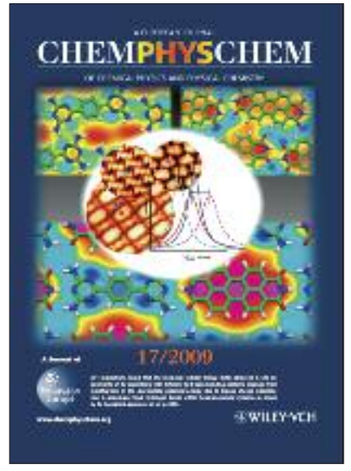
DFT calculations reveal that the molecular orbital energy shifts observed in STS experiments of 2D assemblies with different hydrogen-bonding patterns originate from modifications in the electrostatic potential energy due to a bipolar charge redistribution in anisotropic triple hydrogen bonds within heteromolecular systems.

Chemical bonding is intimately related to the valence electronic structure, but changes in the local molecular orbital structure due to different hydrogen-bonding environments in bi-dimensional assemblies have not been explored in detail so far. In ref. [1], by comparing distinct hydrogen-bonding configurations for two molecular species, we have provided the spectroscopic fingerprint of such changes, which are explained in terms of charge polarization at the molecular scale induced by anisotropic triple hydrogen bonds.

We have studied the unoccupied electronic states of mono- and bicomponent assemblies of 1,4-bis-(2,4-diamino-1,3,5-triazine)-benzene (BDATB) and 3,4,9,10-perylenetetracarboxylic diimide (PTCDI) on Au(111), by combining low-temperature scanning tunneling spectroscopy experiments and density functional theory based calculations. Homomolecular BDATB and PTCDI assemblies exhibit a twofold frontal hydrogen-bonding configuration, while the heteromolecular BDATB-PTCDI system is stabilized by a threefold frontal hydrogen-bonding array [Fig. 1a)-c)]. It turns out, that when comparing the dI/dV spectra of pure and mixed systems, that is in going from the frontal twofold to the threefold hydrogen-bonding configuration, quite large energy shifts are observed. BDATB peaks present an upward shift, whereas PTCDI peaks shift downwards. The origin of these shifts is understood thanks to first-principles DFT calculations of the free-standing molecular layers. We find that the electrostatic potential energy around each molecular species is clearly modified due to an effective bipolar charge redistribution induced in the anisotropic tripe hydrogen bonds within the heteromolecular systems. In other words, in going from the pure systems to the mixture the electrostatic potential at BDATB gets more repulsive and the potential at PTCDI gets more attractive, finally leading to the observed upward and downward energy shifts.

STS signatures of complementary H-bonds formation are shown.

Our results do not only provide detailed new insight into the hydrogen-bonding interactions driving the self-assembly, but also provide the perspective to control and design the electronic properties of hydrogen-bonded supramolecular architectures.



Inside cover ChemPhysChem: Ref. [1] featured in the inside cover of ChemPhysChem 10th volume. The picture in the center shows schematically the observed energy shifts for STS spectra taken on different molecules, and corresponding experimental STM images. The colored graphs in the background correspond to the electrostatic potential energy distribution depicting its modification in going from the pure systems to the mixed system.

Local polarization at the molecular level explain the observed energy shifts.

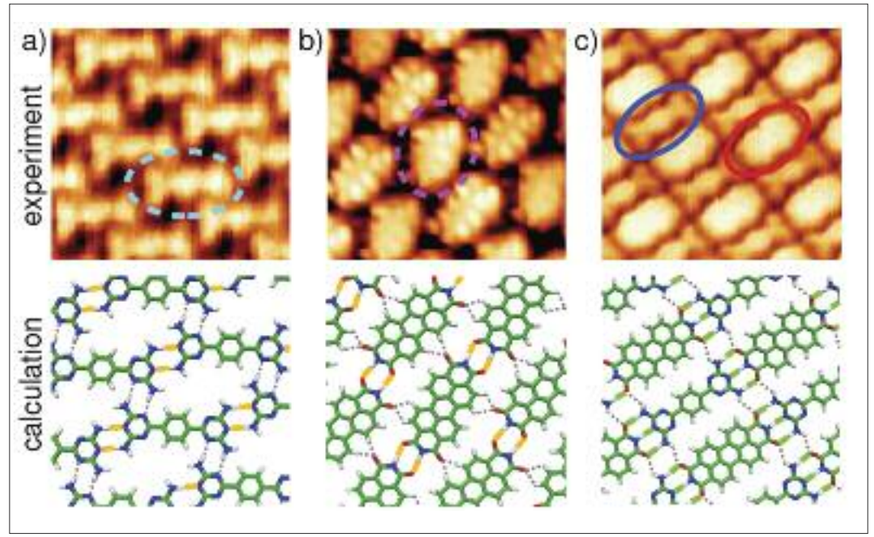


Figure 1. a)-c) STM images from mono- (pure) and bicomponent (mixture) supramolecular self-assemblies on Au(111): a) pure BDATB (1.6 V, 0.03 nA), b) pure PTCDI (-1.7 V, 0.10 nA) and c) BDATB-PTCDI binary mixture (-0.3 V, 0.10 nA). The corresponding bottom panels show the calculated relaxed structures of each periodic system, which illustrate the twofold frontal hydrogen-bonding configuration (marked in yellow) of the monocomponent systems adn the threefold frontal hydrogen-bonding pattern of the mixture (marked in green).

The pathways of micelle formation

Reidar Lund, Lutz. Willner, Michael Monkenbusch, Pierre Panine,
Theyencheri Narayanan, Juan Colmenero and Dieter Richter
Physical Review Letters, 102, 188301 (2009)

For the first time, the spontaneous self-assembly of micelles are captured using small angle x-ray scattering techniques with a time resolution in the millisecond range. Detailed modelling shows that the data can be satisfactorily described using a rather simple nucleation and growth model where only one chain can be added at time.

In material science and physical chemistry, self-assembly is an important route for manipulation and control for a rational design of nanostructures. Synthetic amphiphilic block copolymers belong to the family of self-assembling systems which, apart from the spontaneous self-assembly property, exhibits tuneablity via control over block composition, molecular weight and cosolvents. In order to fully understand and exploit the properties of self-assembled structures, the pathways of their formation need to be understood. So far, such a study has been exceedingly difficult if not impossible because of the lack of experimental techniques that are able to capture and resolve the early stage of this rapid process.

Here we have taken advantage of advances in modern synchrotron radiation instrumentation and for the first time been able to capture and describe how self-assembly of amphiphilic block copolymers takes place in real time using the ID02 beamline at ESRF. Using block copolymers that are molecularly dissolved in a organic polar solvent, micellization can be induced by simply adding water. This process has been observed experimentally using the set-up illustrated in Figure 1, where a stopped flow apparatus is used to assure rapid mixing of the two components in a millisecond time scale. The reaction itself is monitored directly using fast X-ray shots with some millisecond time resolution that allowed the observation of the birth and growth of the micellar aggregates in time. The obtained scattering curves contain relevant structural characteristics of the micelles, such as sizes, volumes and density profiles.

The observed behavior can be quantitatively reproduced using a kinetic model involving insertion and expulsion of single block polymer chains (unimers) by combining classical nucleation and growth theory with the thermodynamic expression expected for block copolymers. It was assumed that only single molecules (unimers) can be taken up for each cluster at a time. As seen in the simultaneous fits in Figure 2 a), the model agrees very well with the experimentally observed growth. In the beginning a very fast initial nucleation, or primary micellization, that consumes all the unimers can be observed. The final stage of the micellization is governed by unimer exchange following a type of ripening mechanism where small micelles slowly dissolve to provide further unimers and the larger ones gradually grow. This goes on until the micelles approach the shallow minimum of the equilibrium size and the distribution narrows to reflect the thermodynamic equilibrium. This scenario is summarized schematically in Figure 2 b).

The excellent agreement with this model strongly suggests that the most effective way for micelle formation is simple addition of unimers from a homogeneous solution. This insight gives novel and valuable information of not only the formation and kinetic pathways of these structures but also the stability and lifetime of metastable nano-particles. This knowledge may be utilized for facile predictive design and manipulation of nano-structures in e.g. medicine or material science.

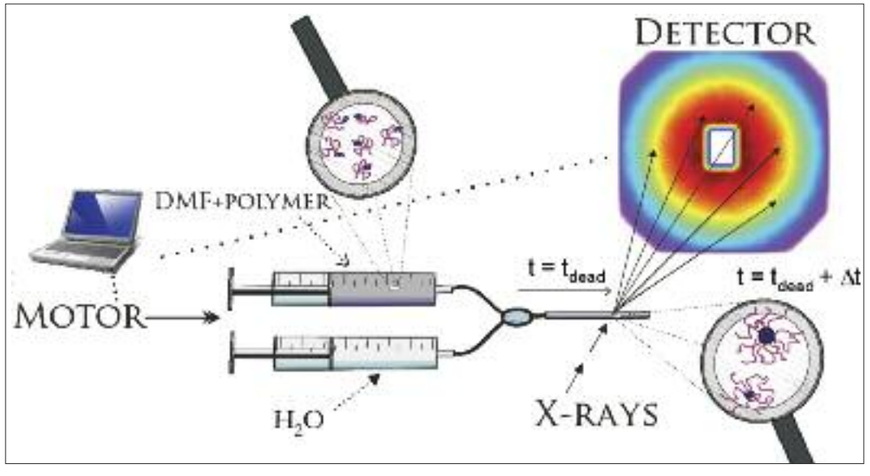


Figure 1. Experimental set-up: The stopped flow set-up consists of two motorized syringes containing the reservoirs with polymer solution and water respectively. Equal amounts of the solution are mixed and then transferred to the observation capillary within a few milliseconds- thereafter the growth is detected by x-ray pulses.

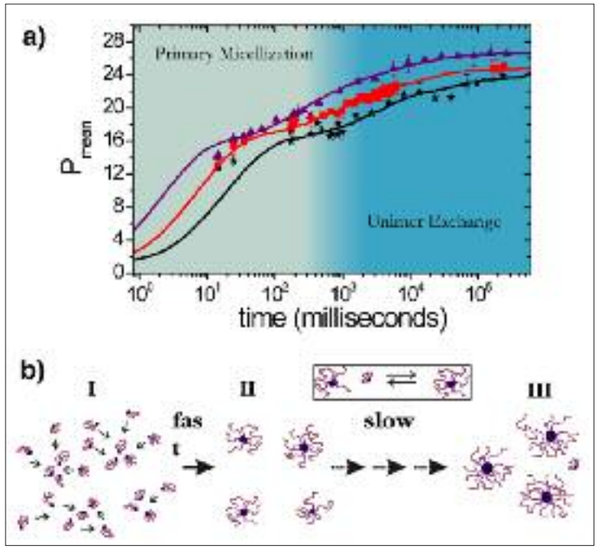


Figure 2. (a) Time evolution of the mean aggregation number of micelles (Pmean) for different concentrations of the block copolymer. Continuous lines represent fits to the nucleation and growth model. (b) Schematic representation of the micellization process involving a fast nucleation in which the unimer concentration is depleted and a slow growth to micelle/unimer.

Micelles seem to grow in a stepwise fashion where only one molecule is inserted or removed at a time.

Quantum oscillations in coupled two-dimensional electron systems

S. Mathias, S. V. Eremeev, E.V. Chulkov, M. Aeschlimann, and M. Bauer
Physical Review Letters 103, 0268 02 (2009)

Two prominent examples of electronic systems with reduced dimensionality are Shockley-type surface (SS) states of the (111) oriented noble metal surfaces and quantum-well (QW) states in ultrathin metallic films. The former are states which are restricted to the outermost atomic surface layers and therefore represent an almost ideal example for two-dimensional electron systems. QW states evolve by the confinement of electrons in ultrathin metal films. QW states arise as the standing electron waves supported by the film and many properties depend critically on the film thickness. These properties show a clear oscillatory dependence on the film thickness (quantum oscillations). We show that such a quantum oscillatory behaviour can efficiently be transferred between two coupled two-dimensional electron systems. Experimentally and from microscopic calculations we have studied the electron-phonon (e-ph) coupling parameter λ of the Ag(111) SS band as modified by the thickness of a supporting silver QW. By means of photoelectron spectroscopy we have identified clear oscillations in λ as a function of QW thickness. Our microscopic model calculations quantitatively reproduce these experimental findings.

In Figure 1 we show experimental and theoretical λ values of the SS state as a function of the thickness of the silver QW between 15 monolayers (ML) and 40 ML. The variations in λ of both data sets follow a clear oscillatory behavior. It exhibits an amplitude of ~ 0.02 and an oscillation period of about 10-12 ML. The slightly varying thickness scale between experiment and theory is due to uncertainties in the determination of the film thickness in the experiment. The overall lower values of the theoretical data (~0.1) were expected, since the calculations do not include the constant background of phonon mediated scattering processes from the Cu substrate as well as from defects scattering contribution to the total linewidth. As mentioned above, oscillations in distinct properties of a QW are a rather common behavior arising from the quantization of the electron spectrum in the QW. Our results provide for the first time evidence that such a quantum-oscillatory behaviour can efficiently be transferred to another low-dimensional electronic system that is coupled to the QW. Below we identify the relevant peculiarities which are responsible for this transfer process.

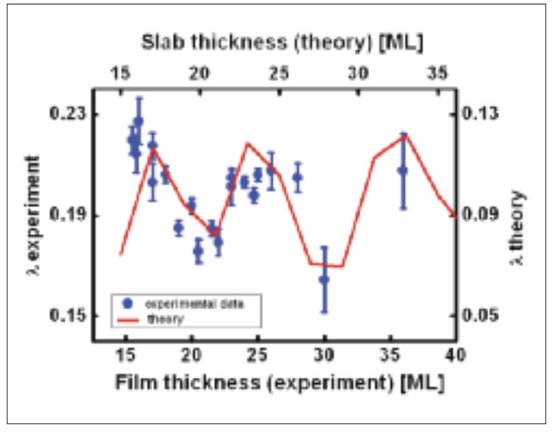


Figure 1. Electron phonon coupling parameter for the SS state as a function of Ag film thickness. Blue dots show the experimental data, the red line the theoretical data.

Figure 2 displays results from a calculation of apartial λ of the surface state ($\lambda_{gap\text{-}QWS}$) which considers exclusively QW states in the energy regime of the Cu(111) substrate band gap (below 850 meV binding energy). At distinct film thicknesses an additional QW state moves into resonance with the Cu band gap and, hence, increases the number of QW states, which affect $\lambda_{gap\text{-}QWS}$, by one. The appearance of this additional QW state within the band gap is equivalent to a sudden localization of the QW wave-function in the Ag-film. Such localization takes place for instance at a slab thickness of 22 ML and obviously contributes considerably to the amplitude of the second oscillation maximum of $\lambda_{gap\text{-}QWS}$. The magnitude of $\lambda_{gap\text{-}QWS}$ is, however, by far too small to explain the total amplitude of λ_{SS} and accounts for only 10% of the observed experimental value. The overlap of the SS wave function with QW states outside of the Cu(111) band gap accounts for the remaining 90% of the amplitude. The latter, the sum over oscillations of all partial contributions, is obviously a crucial factor responsible for the pronounced oscillations in λ_{SS}. However, these oscillations cannot be explained by a simple overlap effect. The localization of the SS state wave-function at the surface of the quantum-well is essential ingredient for the observed oscillatory behavior. Another significant ingredient is the gradient of the one-electron potential which enhances the oscillation amplitude of λ_{SS}.

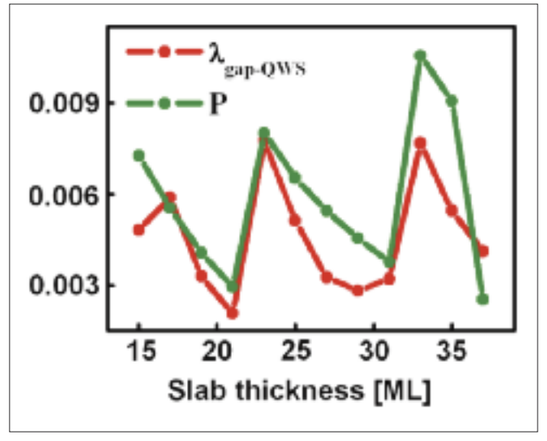


Figure 2. Partial λ to the electron phonon coupling parameter of the SS state from the QW states localized in the Cu(111) band gap as a function of film thickness and overlap P of corresponding wave functions.

Our microscopic model calculations quantitatively reproduce these experimental findings.

Passing current through touching molecules

G. Schull, T. Frederiksen, M. Brandbyge, and R. Berndt
Physical Review Letters 130, 206803 (2009)
Paper selected for "Editor's Suggestion" and American Physical Society's "Physical Review Focus"

The charge flow from a single C_{60} molecule to another one has been probed. A scanning tunneling microscope (STM) was used to first pick up a single C_{60} molecule with the tip and thereafter to approach it to a second molecule with atomic-scale precision. This novel method allows for detailed studies of intermolecular charge transport, which is crucial for the realization of efficient electronic devices, sensors, and solar cells based on molecular materials.

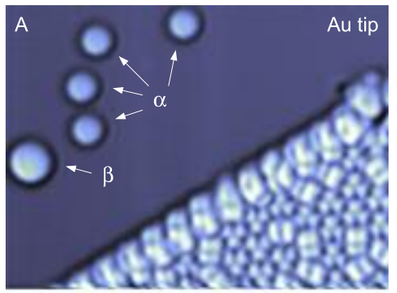
The performance of modern electronics increases steadily on a fast pace thanks to the ongoing miniaturization of the components. However, severe problems arise due to quantum-mechanical phenomena when conventional structures are simply made smaller and reach the nanometer scale. Therefore current research focuses on the so-called bottom-up approach: the engineering of functional structures with the smallest possible building blocks, namely single atoms and molecules. These efforts have resulted in a detailed insight into the transport properties of individual nanoscopic objects. A critical issue is now to understand and control the charge transport from one molecule to another one.

In this work the intermolecular charge transport through a C_{60}-C_{60} bridge was investigated for the first time. In order to realize this setup a technique to transfer a C_{60} molecule to the tip of an STM was devised. Examples of images acquired before and after the transfer of the molecule to the tip is shown in Figure 1. The molecular orientation could be inferred via adatoms deposited on clean areas of the metal substrate. Hereafter the C_{60}-functionalized tip was approached to a second molecule with a precision of a few picometers. During this controlled approach the researchers measured the electrical current that flows between the two molecules, which depends critically on the distance between the molecules. Ultimately, the molecules touch each other and the current attains its maximum value.

The investigation revealed that the electrical current does not flow easily between the two touching C_{60} molecules - the conductance is 100 times smaller than for a single molecule. This finding is interesting for future devices with closely packed molecules as it indicates that leakage currents between neighboring circuits will be controllable.

The experimental findings are strongly supported by first-principles transport simulations carried out at the DIPC. These calculations reproduce the experimental results and identifies the role of the intermolecular link in the conductance of the C_{60}-C_{60} bridge (Figure 2). The theory further gives access to the distance-dependent nature of the electrical current and predict the evolution of the transport properties for longer chains of suspended C_{60} molecules.

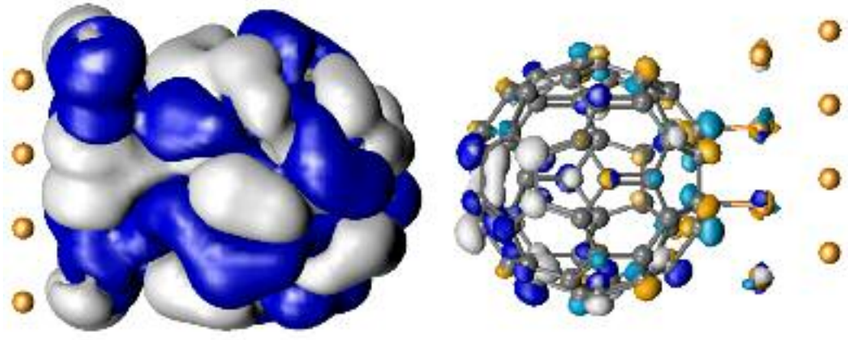
The extreme precision of manipulation and control of single molecules presented in this work open up a new route for exploring other promising molecules to address the influence of the molecule-molecule interactions on intermolecular charge transport. The deeper understanding of this current is an essential step towards novel molecular nanoelectronics.



STM images of Au(111) partially covered with C60 molecules (lower right) obtained with (A) a metal tip and (B) a C60-tip over the same area. Gold adatoms (α) and a small gold cluster (β) of two or three atoms are discernable. After imaging with the C_{60}-tip it was used to make contact to another C_{60} molecule in order to study the conductance of a C_{60}-C_{60} bridge.

Understanding intermolecular charge transport is essential towards novel molecular nanoelectronics.

Image published on the cover of *Physical Review Letters*



Electron current through two C_{60} molecules contacted with metal electrodes. The isosurface of the electron wave (incoming from the left) extends with large amplitude over the first C_{60} molecule but is reflected at the interface between the two C_{60} cages. The strongly attenuated outgoing wave (to the right) illustrates that the low transmission probability (and correspondingly the relatively low conductance) of the C_{60}-C_{60} bridge is due to the intermolecular link.

Angle-resolved photoemission study of the graphite intercalation compound KC8: a key to graphene

A. Grüneis, C. Attaccalite, A. Rubio, D.V. Vyalikh,
S.L. Molodtsov, J. Fink, R. Follath, W. Eberhardt, B. Büchner, and T. Pichler
Physical Review B 80, 075431 (2009)

Idealized graphene is a two-dimensional sheet of carbon. The electrons in graphene behave like massless Dirac particles that appear in the electronic band structure as gapless excitations with a linear dispersion—the "Dirac cone." However, in real life, graphene is never perfectly flat and may interact with the substrate that supports it, which significantly alter graphene's electronic properties. Invariably, these effects open a gap that limits the observation of relativistic physics in graphene.

Every week there are numerous papers explaining the exotic features of graphene, a single layer of carbon atoms arranged in a honeycomb lattice. Due to the honeycomb lattice, electrons in graphene behave as massless particles. In ideal, freestanding graphene, electrons can move through the crystal without scattering with carbon atoms. This is very much the way that light propagates (with a velocity that is only 1/300 of the speed of light). Therefore electrons in graphene are described by the Dirac equation – indeed this is something very unique in condensed matter physics. Unfortunately this ideal view of graphene contrasts with experimental evidences where coupling with the substrate or to adjacent graphene layers spoils the massless Dirac Fermion behaviour predicted from the theory. In this case the substrate interaction causes the electronic structure to open up a gap and the electrons to acquire a finite mass. Then they are no longer described by the Dirac equation.

In this article researchers from the IFW in Dresden, Germany, and collaborators from Austria and Spain observe the full Dirac cone dispersion, expected for isolated graphene, in an intercalated graphite compound KC8 using angle resolved photoemission spectroscopy. The potassium ions move in between individual graphene sheets (this process is also known as intercalation) thereby separating adjacent graphene layers apart and cancelling their interaction. The KC8 crystal consists of individual graphene sheets separated by layers of potassium. Combining angle-resolved photoemission spectroscopy measured at the BESSY synchrotron in Berlin and theoretical calculations from DIPC and the European Theoretical Spectroscopy Facility, they unravelled the full experimental Dirac cone of electrons in graphene revealing an anisotropic linear dispersion in all directions, the same way how light propagates (see Figure). It turns out that there is a complete charge transfer from potassium to the graphene layers but there is no Coulomb interaction between the layers. This preserves the Dirac cone dispersion for both the valence and conduction bands, though the doping shifts the Dirac point away from the chemical potential (differently from what is expected for pristine graphene). This allowed them to measure not only the valence bands but also the conduction bands of graphene for a large energy range, not reachable in single layer graphene. State-of-the art electronic structure calculations including electron-electron interactions within the graphene sheets needs to be taken into account to get excellent agreement with experimental. These results provide crucial input to study the electronic and transport properties of isolated graphene, which has hitherto been difficult due to substrate effects.

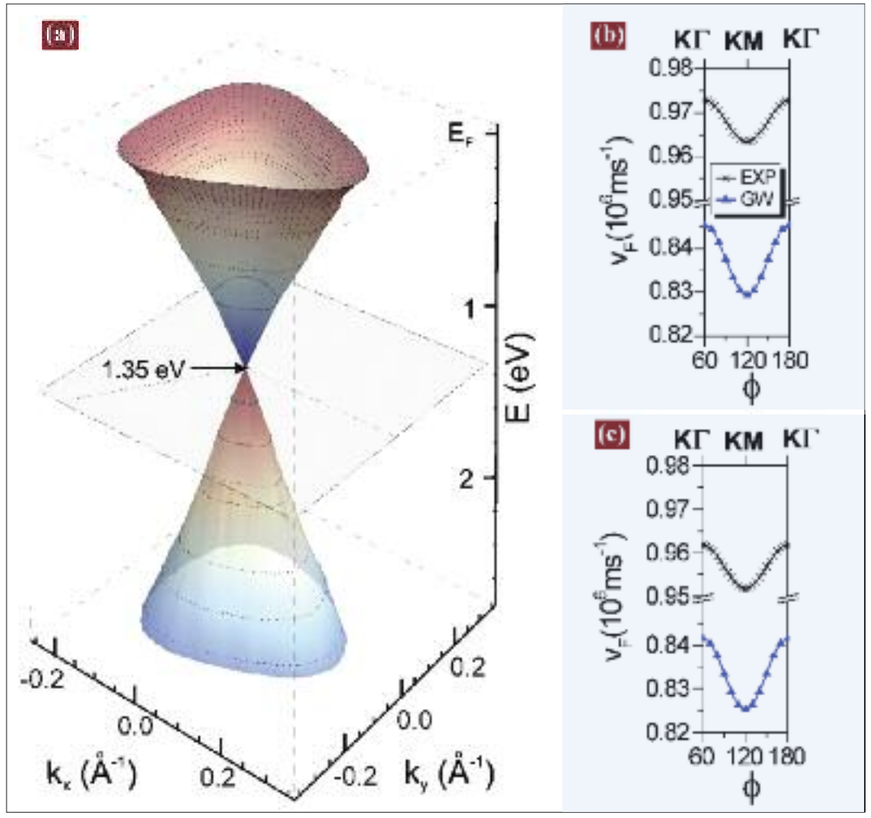


Figure 1. (a) Experimental Dirac cone from the observed photoemission intensity maxima (denoted as dots). Measured and calculated (GW) values of vF for (b) electrons and (c) holes around the Dirac point.

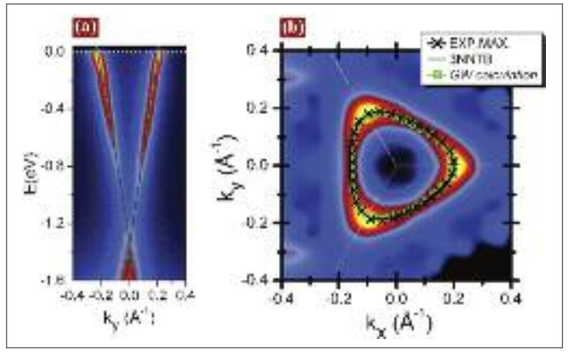


Figure 2. (a) ARPES scan measured close to the ky direction along with the bare-band dispersion (black) and the GW calculation for rigidly doped graphene (green).
(b) Symmetrized equi–energy contour for E=0.24 eV and maxima (crosses) along with a tight-binding fit and the GW ab-initio calculations.

Dirac cone revealed.

Acousto-plasmonic hot spots in metallic nano-objects

N. Large, L. Saviot, J. Margueritat, J. Gonzalo,
C.N. Afonso, A. Arbouet, P. Langot, A. Mlayah and J. Aizpurua
Nano Letters 9, 3732 (2009)

We introduce the concept of acousto-plasmonic dynamics of metallic nano-objects. Acousto-plasmonic interactions still present several theoretical challenges to correctly interpret the Raman-Brillouin scattering. Several works have been devoted to the study of shape, size and environment effects on the surface plasmons whereas there are only few studies of their dynamical properties such as coupling mechanisms to the acoustic vibrations.

We experimentally observe unexpectedly strong acoustic vibration bands in the Raman scattering of silver nanocolumns (NCIs), usually not found in isolated nano-objects. The frequency and the polarization of this unexpected Raman band allow us to assign it to breathing-like acoustic vibration modes (blue arrow in Figure 2). To understand this "anomalous" Raman scattering, we address a theoretical and experimental study of the interactions between acoustic vibrations (upper part of Figure 1) and surface plasmons (lower part of Figure 1). The modulation of the surface plasmon nearfield (lower part of Figure 1) allows for the interpretation of experimental Raman-Brillouin spectra in these NCIs.

Based on full electromagnetic near-field calculations coupled to the elasticity theory, we introduce a new concept of "acousto-plasmonic hot spots" which arise here because of the indented shape of the NCIs. These hot spots combine both highly localized surface plasmons and strong shape deformation by the acoustic vibrations at specific sites of the nano-objects. In order to investigate this new concept, we integrate the Boundary Element Method for the electromagnetic calculations and the elasticity theory by the means of the RUS method for the vibrational calculations, which allows calculating the modulation of the surface plasmon polarization for these acoustic vibrations.

We show that the interaction between breathing-like acoustic vibrations and surface plasmons at the "acousto-plasmonic hot spots" is strongly enhanced, turning almost silent vibration modes into efficient Raman scatterers. The indentations of the silver NCIs are responsible for the strong localization of the surface plasmon nearfield and its modulation by breathing-like acoustic vibrations (Figure 2). The concepts, the numerical and experimental approaches developed here are not specific to indented NCIs and can be extended to other isolated nano-objects exhibiting strong field localization, dimers and more complex metallic nanostructures combining size, shape and interaction effects.

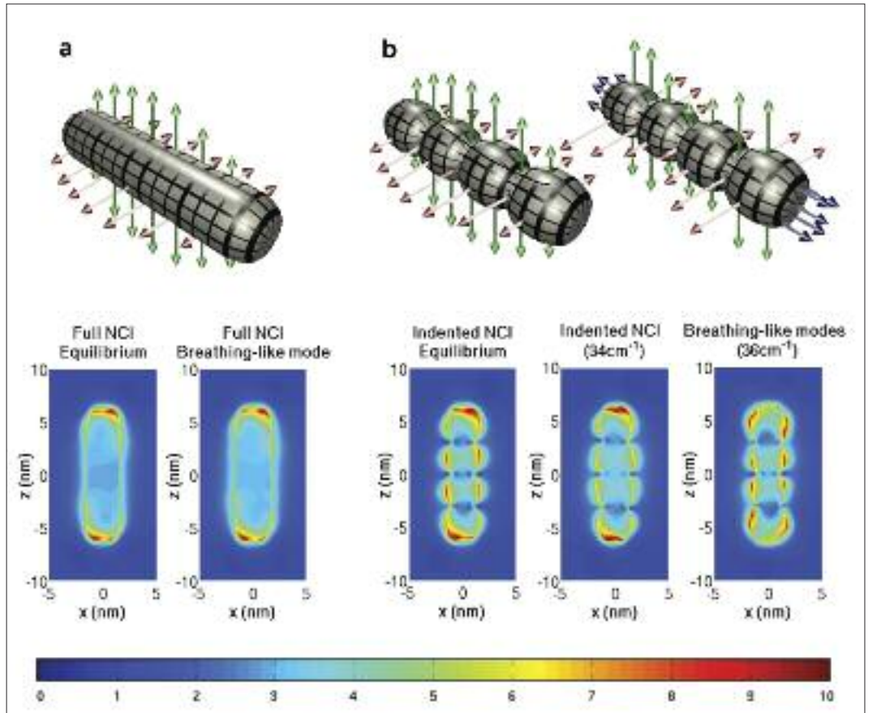


Figure 1. Upper part: Displacement field associated to the breathing-like acoustic vibrations for (a) a full NCI and (b) an indented NCI. Lower part: Nearfield disctribution for (a) a full NCI and (b) an indented NCI at the equilibrium (without vibrations) and deformed by the breathing-like acoustic modes.

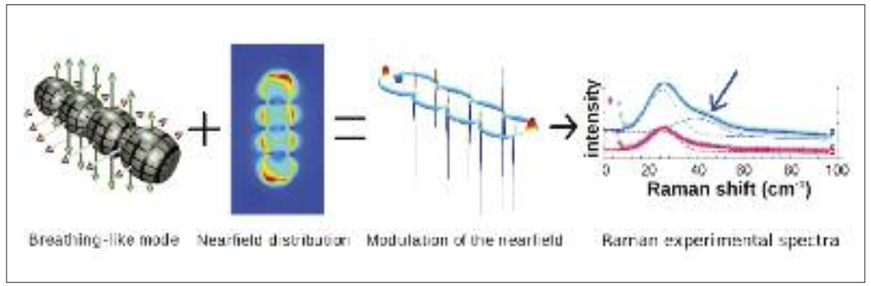


Figure 2: Breathing-like acoustic vibrations modulate the surface plasmon nearfield of a silver indented NCI and induce a relative modulation of the surface plasmon polarization $\delta_{vib}P(r)/P_0(r)$. This modulation is responsible for the activation of the "anomalous" acoustic band (marked with the blue arrow) in the Raman spectrum.

Supramolecular environment-dependent electronic properties of metal-organic interfaces

Dimas G. de Oteyza, Juan María García-Lastra, Martina Corso, Bryan P. Doyle,
Luca Floreano, Alberto Morgante, Yutaka Wakayama, Angel Rubio and J. Enrique Ortega
Advanced Functional Materials 19, 3567 (2009)

In this work, we address the changes in the electronic structure of donor-acceptor molecular mixtures with respect to that of the isolated components. The changes arise as a consequence of the modified interactions in the supramolecular layers, whose understanding is crucial for a better control of the self-assembly processes on surfaces.

Charge transfer processes between donor–acceptor complexes and metallic electrodes are at the heart of novel organic optoelectronic devices such as solar cells. In fact, molecular dyads allow the development of new architectures according to a win-win design strategy, thanks to the varied properties offered by organic semiconductors. On the one hand, the optical sensitivity of the photovoltaic cell can be tuned to the environmental light conditions by appropriate choice of the molecular pair. On the other hand, the intermolecular interactions can be trimmed by chemical functionalization of the respective molecules, in order to optimize the molecular coupling in the supramolecular assembly. The bottleneck of this emerging technology is represented by the interface with the supporting metal contact, where the charge signal is extracted. Most studies on interfacial electronic properties, which are crucial factors for charge carrier injection/extraction and thus for the functionality of organic based optoelectronic devices, have been performed on model single-component molecular layers on metals. In spite of the expected key role of nanostructured donor–acceptor systems in future development of organic devices, these have been mostly studied from a structural and only scarcely from an electronic point of view. Here we show that the charge transfer and the chemical properties of metal-organic interfaces based on single component organic layers cannot be naively extrapolated to the new molecular environments of supramolecular architectures, such as donor–acceptor binary assemblies. As a consequence, a detailed atomistic understanding of the hybrid junction between electrode and organic mixture (both from an electronic and structural point of view) is required for a rational design of functional donor–acceptor nanostructures with optimized properties.

Our study focused on binary supramolecular nanostructures on copper (111) surfaces, comprising perfluorinated copper-phthalocyanines (F_{16}CuPc) and diindenoperylene (DIP). The electronic and crystalline properties have been addressed by means of scanning tunnelling microscopy (STM), synchrotron radiation spectroscopy measurements including valence-band (UPS), high resolution core-level photoelectron spectroscopy (XPS), as well as near edge X-ray absorption fine structure (NEXAFS), and state-of-the-art ab-initio calculations.

Figure 1. STM images depicting the crystalline structure of single component DIP, F_{16}CuPc as well as of binary layers. Superimposed on the images are the projected density of states on the respective occupied and unoccupied molecular orbitals closest to the Fermi edge. Their pronounced change of width gives evidence of the modified electronic coupling with the substrate in the mixed layer.

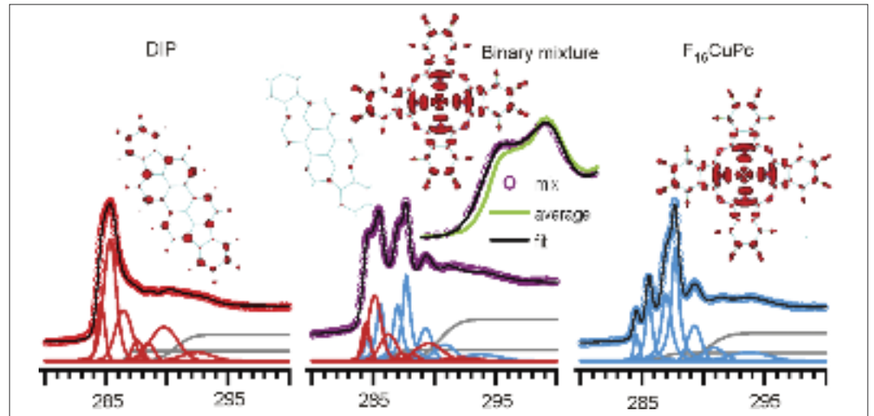


Figure 2. Experimental (symbols) and fitted (lines) C K-edge NEXAFS spectra of single component DIP, F_{16}CuPc and binary layers, together with the fit components. For the binary mixture, a zoom into the absorption edge region evidences the shift of the experimental spectra (in particular of the DIP components) with respect to the expected curve (average of F_{16}CuPc and DIP spectra) if no electronic changes took place in the mixture. Additionally shown are the calculated differences in electronic density with respect to the isolated molecules for F_{16}CuPc and DIP in the single-component and binary layers. The major changes upon molecular mixture take place for DIP, showing a reduced charge transfer.

Upon deposition of both molecules on the clean surface, these mix into a highly crystalline binary layer (Fig. 1), independently of whether the molecules are co-deposited or evaporated sequentially. The driving force behind this pronounced tendency to mix can be found in the greatly enhanced intermolecular interactions arising from the formation of multiple C-H···F-C hydrogen bonds in the binary layers. Most interestingly, the modified intermolecular interactions are accompanied by changes in the electronic coupling between molecules and substrate. In reference to the associated single component layers, the new supramolecular environment of the binary mixture causes the donor molecule (DIP) to decouple electronically from the metal surface, while the acceptor (F_{16}CuPc) suffers strong hybridization with the substrate (Fig. 1). The former causes the DIP-Cu(111) charge transfer to decrease, as evidenced by XPS and NEXAFS, and further supported by theoretical calculations (Fig. 2). UPS measurements and calculations also show how the $d_{3z^2-r^2}$ –like wave-functions of the Cu atoms in close contact with the organic overlayer hybridize with the F_{16}CuPc in the binary layer.

With this work we shed new light on the complex correlations between intermolecular and molecule–substrate interactions, and thereby take a step forward towards a better understanding of the self-assembly processes on surfaces.

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Berman OL, Gumbs G, and Echenique PM.
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Eiguren A, Ambrosch-Draxl C, and Echenique PM.
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A three-dimensional numerical study.
Teperik TV and Borisov AG.
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Men'shov VN, Tugushev VV, Caprara S, Echenique PM and Chulkov EV.
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Gruneis A, Serrano J, Bosak A, Lazzeri M, Molodtsov SL, Wirtz L, Attaccalite C, Krisch M, Rubio A, Mauri F,
and Pichler T.
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Theoretical and experimental study of the Au (111) surface state.
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Lifetimes of quantum well states and resonances in Pb overlayers on Cu(111).
Zugarramurdi A, Zabala N, Silkin VM, Borisov AG, and Chulkov EV.
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Silkin VM, Zhao J, Guinea F, Chulkov EV, Echenique PM, and Petek H.
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and Temmerman WM.
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Two-photon photoemission spectroscopy and electronic structure theory.
Achilli S, Trioni MI, Chulkov EV, Echenique PM, Sametoglu V, Pontius N, Winkelmann A, Kubo A, Zhao J,
and Petek H.
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Polarization-induced renormalization of molecular levels at metallic and semiconducting surfaces.
Garcia-Lastra JM, Rostgaard C, Rubio A, and Thygesen KS.
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ing functions.
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trends across binding regimes.
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Brun C, Hong IP, Pattthey F, Sklyadneva IY, Heid R, Echenique PM, Bohnen KP, Chulkov EV, and Schneider WD.
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Low-coordination phases of both crystalline and fluid states of alkali metals under extreme conditions of high and low densities, respectively.
March NH, and Angilella GGN.
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The induced charge density at the origin.
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Borisova SD, Rusina GG, Eremeev SV, and Chulkov EV.
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Nechaev IA, and Chulkov EV.
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Properties of quasiparticle excitations in FeCo ferromagnetic alloy.
Nechaev IA and Chulkov EV.
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Effect of point defects on the temperature dependence of the Linewidth of a surface electronic state on the Au(111) surface.
Eremeev SV and Chulkov EV.
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Ab initio GW calculations of the time and length of spin relaxation of excited electrons in metal with inclusion of the spin-orbit coupling.
Zhukov VP and Chulkov EV.
Physics of the Solid State 51, 2211 (2009).

Spin-split excitation gap and spin entanglement of a pair of interacting electrons in a quantum dot.
Gumbs G, Huang DH, Blumenthal MD, JWright S, Pepper M, and Abranyos Y.
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Cluster crystals in confinement.
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Inelastic X-ray scattering and first-principles study of electron excitations in MgB2.
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STM study of di-indenoperylene molecules on Cu(100) surfaces: mobility, stability and epitaxy.
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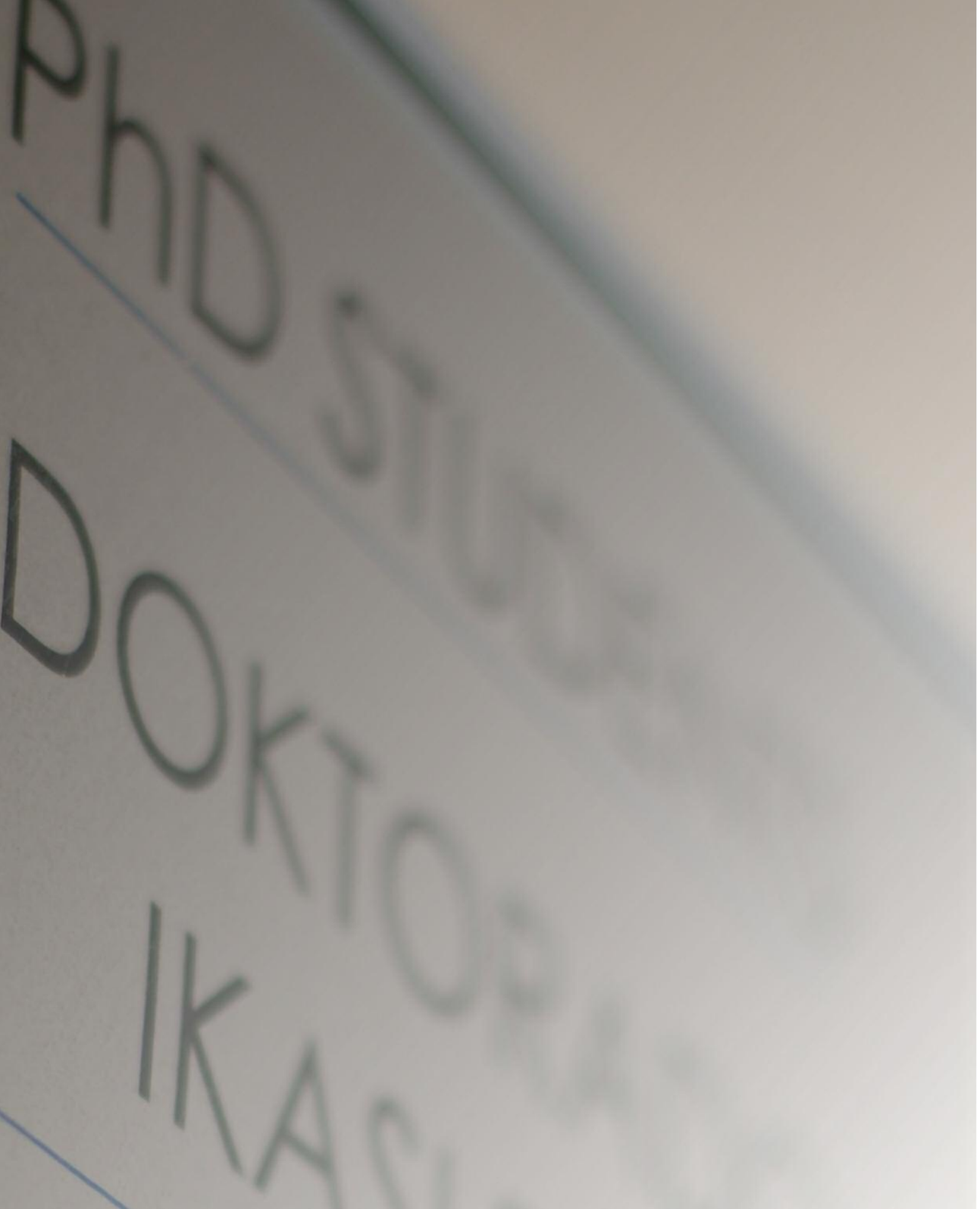

Researchers

Fellows Gipuzkoa

Dr. Javier Aizpurua Iriazabal
National Institute of Standards and Technology, USA
01/01/2004–31/07/2008
Electronic and optical properties of metal nanostructures and semiconductor low-dimensional systems. Nanooptics for field-enhanced microscopies and spectroscopies.

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. Asier Eiguren Goienetxea
University of Leoben, Austria
11/06/2007–05/10/2009
Study of the electron-phonon interaction in strongly correlated and strong coupling systems. Calculation of electron-phonon sensitive thermodynamic properties including, heat capacity, different susceptibilities and charge and spin transport in low dimensional systems. Implementation of the Wilson's numerical renormalization group method to electron-phonon interaction. Comparative study of the limitations of the perturbative approaches in relation to the renormalization group. Superconductivity.

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, non-equilibrium 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.

Postdoctoral Positions

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

Dr. Iñaki Silanes Cristóbal
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/01/2007–15/03/2008
Surface-assisted assembly of two dimensional molecular networks with different coordination symmetry. Study of oxygen adsorption on several Pophyrins (Fe and Mg coordinated). Molecular Switches based on different conformational change induced architectures.

Dr. Martina Corso
University of Zurich, Switzerland
02/01/2007–16/10/2009
Boron nitride nanomesh: a peculiar self-assembled nanostructure.

Dr. Gisela Bocan
Universidad de Buenos Aires, Argentina
01/02/2007–07/02/2009
Gas-surface systems. Dynamics of diatomic molecules impinging on metallic surfaces. Dissociative adsorption and Scattering. Exchange-correlation and DFT calculations. Potential Energy Surface Calculations.

Dr. Thomas Frederiksen
Technical University of Denmark
01/05/2007–29/02/2008
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. Daniel Bozi
ICMM, CSIC, Madrid, Spain
01/08/2007–18/12/2008
Study of the properties of the low-dimensional systems that can be realized by loading ultra cold atomic gases in optical lattices or other types of very anisotropic traps. Study of the absence of thermalization in integrable realizations thereof. Calculation of corrlation properties in strongly interacting systems. Study of the atom-surface interactions, the Casimir Effect in and out of equilibrium.

Dr. Alejandro Reyes Coronado
Universidad Nacional Autónoma de México
30/08/2007–31/08/2009
Optical response of resonant metallic nanostructures in surface-enhanced microscopy and spectroscopy.

Dr. Dimas Garcia de Oteyza Feldermann
Max Planck Institute for Metal Research, Stuttgart, Germany
01/09/2007–Present
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–Present
Plastic deformation of gamma phase isotactic polypropilene in the plane-strain compression.

Dr. Dusan Racko
Polymer Institut Slovak Academy of Sciences, Bratislava, Slovak Republic
03/09/2007–Present
Molecular dynamics simulations in polymers.

Dr. Mario Piris Silvera
University Erlangen-Nuremberg, Germany
01/10/2007–03/05/2008
Natural Orbital Functional Theory (NOFT). Correlation studies by means of electron-pair density functions. Description of van der Waals interactions. Characterization of ZnS nanostructures endohedraly doped with transition metals. Study of ZnS, BN and Sn12 nanoclusters and solids.

Dr. Nicolay Zaytsev
Sibirian Institute of Physics and Technology, Tomsk, Russia
04/10/2007–06/08/2009
Study of spin dependent electronic structure and spin-orbit interaction at clean metal surfaces and at surfaces with adsorbate. This activity has attracted much attention last years both experimentally and theoretically. The study of electronic structure of carbon surface as well as of noble metal and ferromagnetic metal surfaces.

Dr. Maia García Vergniory
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
05/12/2007–31/01/2008
Many body and band structure effects on the interaction between hot electrons and ions with solid surfaces.

Dr. Claudio Horowitz
Centro Atómico Bariloche, Argentina
29/02/2008–28/02/2009
Optimized effective-potential approach to the Kohn-Sham exchange-correlation potential of density-functional theory.

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. René Gaudoin
Rutgers University, New Jersey, USA
01/06/2008–20/02/2009
Diffusion Monte Carlo investigations of electron correlation in bulk systems and solid surfaces.

Dr. Virginie Boucher
University of Lille (ENSCL), France
30/10/2008–Present
Dynamical properties at molecular scale in polymeric materials multi-component and/or nano-structured, combining different experimental techniques and in particular, dielectric and mechanical spectroscopy. There is also the possibility of using also X-rays and neutron scattering.

Dr. Bruno Rousseau
Cornell University, USA
01/11/2008–15/05/2009
Theoretical analysis of pressure induced electronic and superconducting anomalies in simple elements and their alloys.

Dr. Remi Busselez
Universite de Rennes, France
03/11/2008–Present
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. Vito Despoja
University of Zagreb, Croatia
22/02–15/05/2009
Within the present project will be investigated within framework of ab initio time-dependent density-functional theory the properties of excited electrons and holes and collective electronic excitations at the low-energy domain in iron-based metallic systems called pnictides which have been discovered recently and characterized by an elevated critical temperature of the superconducting transition.

Dr. Ludovic Martin
Université Bordeaux1, Talence, France
01/09/2009–Present
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
School of Physical Sciences, Jawaharlal Nehru University, New Delhi, India
07/09/2009–Present
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
University of Basel, Switzerland
01/11/2009–Present
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.

Temporary Contract Positions

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 Saint Petersburg, Russia
17/07/2009–Present
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, San Sebastian, Spain
16/11/2009–Present
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 Fellowships

Remi Vincent
Université Paul Sabatier, Toulouse, France
01/11/2003–30/11/2009
Ions induced electron excitations in ferromagnetic materials. Interaction of ions with metals energy loss and stopping power. Study of metallic clusters. Response function.

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

Iñigo Aldazabal Mensa
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/07/2006–12/08/2008
Electron emission in ion-surface grazing collisions; contributions to the convoy electrons. Wave packet propagation tecniques applied to STM systems.Laser induced electron emission in metallic surfaces.

Martin Brodeck
IFF-FZ, Forschungszentrum Jülich, Germany
01/10/2006–15/04/2008
Molecular dynamics simulations and neutron scattering measurements of the strongly decoupled dynamics which are exhibited by the different components of polyethyleneoxide (PEO)/polymethylmetacrylate (PMMA) blends which can differ up to 12 orders of magnitude in local relaxation times.

Olalla Pérez González
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
02/10/2006–Present
Plasmon excitations in metallic nanoparticles. Optical properties of nanostructured materials.

Xabier Zubizarreta Iriarte
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
16/10/2006–30/09/2008
Electronic structure calculations of metal surfaces with strong spin-orbit coupling.

Yon Sánchez Paisal
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
16/10/2006–09/03/2008
Electronic structure calculations in nanostructured systems with technological applications.

Juan Pablo Echeverry Enciso
Universidad del Valle, Cali, Colombia
28/08/2007–30/06/2008
Study of colective electronic excitations and dinamic of reduced symmetry systems.

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

Nicolas Large
Université Paul Sabatier, France
01/10/2007–Present
Simulations of the optical properties of metallic nano-objects: acoustic phonons - surface plasmons coupling. Raman spectroscopy in low dimensional semiconductor structures.

Sandra Plaza García
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/10/2007–Present
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, Italy
29/10/2007–Present
Molecular dynamics simulations of simple models for glass-forming polymers.

Marina Quijada Van den Berghe
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/11/2007–30/10/2009
Electron dynamics in metal clusters. Study of the size effects in the lifetime of excited electrons in metal clusters. TDDFT calculation of the energy loss in collision processes of charges with metal clusters.

Itziar Goikoetxea Martinez
Universidad Complutense, Spain
01/12/2007–30/06/2008
Non-adiabatic processes in the adsorption of diatomic molecules on metal surfaces.

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

Giuseppe Foti
Universita Mediterranea di Reggio di Calabria, Italia
01/11/2008–30/06/2009
Electronic transport through molecular

Zakaria Mohammed Slimani
Centre Européen de Calcul Atomique et Moléculaire (CECAM), Lyon
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–Present
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
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/12/2009–Present
Transport properties of superconducting weak links in the presence of a rf-field.

Visiting Researchers

Long visits

Prof. Eugene Krasovskii
Universität Kiel, Germany
07/01–30/03/2008
First-principles calculations of collective excitations in bulk metals.

Prof. Joseph R. Manson
Clemson University, USA
06/05–15/08/2008
Theoretical investigations of the microscopic structure and dynamical properties of surfaces.

Prof. Juan José Sáenz Gutierrez
Universidad Autónoma, Spain
01/06–31/07/2008, 01/06–30/07/2009
Nanophotonics. Modeling scanning probe microscopies.

Prof. Wolfgang Schattke
Universität Kiel, Germany
01/10–30/11/2008
Variational Quantum Montecarlo calculations of the electronic properties of solids and surfaces. Theory of photoemission in semiconductors and metals.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Italy
02/06–30/06/2008, 02/10–30/10/2008, 01/06–30/06/2009
Surface phonons and phase transitions.

Prof. Viktor Tugushev
RRC Kurchatov Institute, Moscow, Russia
03/04–27/06/2008
Magnetism in superlattices and spintronics.

Prof. Vladimir Menshov
RRC Kurchatov Institute, Moscow, Russia
15/05–15/08/2008
Confling mechanisms in digital alloys.

Prof. Sergey Eremeev
Institute of Strength Physics and Materials Sciences, Tomsk, Russia
01/06–30/08/2008, 03/07–30/09/2009
Phonons and electron-phonon coupling in quantum-well states of adlayers on metals.

Prof. Philippe Tordjeman
Université Montpellier 2, France
04/02–18/06/2008
Nanodielectric of polymer.

Prof. Amand Lucas
FUNDP, Namur, Belgium
30/09–30/10/2008, 03/09–30/11/2009
Condensed matter physics, surface sciences, electronic and atomic structures of reduced dimensionality systems structural biology.

Dr. Ilya Nechaev
Kostroma State University, Russia
22/06–19/09/2008, 21/06–16/09/2009
Electron excitations in ferromagnetic materials.

Prof. Norman March
University of Antwerpen, Belgium
08/04–08/06/2008, 15/04–14/06/2009
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.

Mbamba Kandi Masakidi
Ecole Nationale Supérieure de Chimie de Lille, France
31/03–15/06/2008
Mechanical and dielectric properties of trans-Poly(isoprene) and its copolymers with styrene.

Prof. Istvan Nagy
Technical University of Budapest, Hungary
02–30/05/2008, 04–27/09/2008,
07/01–06/02/2009, 04–30/05/2009, 01–26/09/2009
Various aspects of correlations in extended fermionic systems; spice-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Doctorand Simona Achilli
CNR, University of Milano-Bicocca, Italy
10/02–10/06/2008
Electronic and magnetic properties of single adatoms on metal surfaces.

Prof. Emilio Artacho Cortés
University of Cambridge, United Kingdom
07/07–7/08/2008
Electronic stopping power in insulators. LDA+U, SIC, exact-exchange in DFT calculations.

Prof. Sergio Caprara
University of Rome Sapienza and Instituto Nazionale per la Fisica della Materia, Rome, Italy
02/04–31/05/2008, 14/04–13/06/2009
Digital alloys.

Dr. Mikhail Otrokov
State University of Tomsk, Russia
01–30/07/2008, 14/06–31/07/2009
Electronic structure of digital alloys.

Dr. Andrey Enyashin
Institute of Solid State Chemistry (Ural Branch of Russian Academy of Sciences) Ekaterinburg, Russia
01–31/08/2008
Composites of inorganic nanotubes and cement.

Dr. Andrey Borissov
Université Paris Sud, France
07–31/07/2008
Time-dependent density functional theory and wave packet propagation methods.

Prof. Arthur Ernst
Max Planck Institut of Microstructures, Germany
01–31/07/2008
Magnetism from first principles: a multiple scattering approach.

Prof. Malcolm Stott
Queen's University, Kingston, Canada
30/12/2008–31/01/2009
2D electron gas.

Doctorand Luca Maini
Universitá di Milano-Bicocca, Italy
01/02–31/07/2009
Simulations of photonic crystals and photonic nanostructures.

Dr. Yuri Koroteev
Tomsk State University, Russia
09/03–10/05/2009
First principles calculations of electronic structure and quasiparticle lifetimes in metals.

Dr. Svetlana Borisova
Physics and Materials Science,
Russian Academy of Sciences, Tomsk, Russia
09/03–10/05/2009
Phonones in metal adlayers.

Prof. Vladlen Zhukov
Ural Branch of Russian Academy of Sciences,
Ekaterinbourg, Russia
14/03–13/06/2009
Electron dynamics in oxides: electron-electron and electron-phonon mechanisms of decay of excited electrons.

Dr. Vladimir Meñshov
RRC Kurchatov Institute, Moscow, Russia
14/05–14/08/2009
Confling mechanisms in digital alloys.

Dr. Silvana Botti
Ecole Polytechnique, Palaiseau, France
15/05–15/06/2009
Theoretical modeling of photovoltaic materials.

Prof. Nikolay Kabachnik
Institut für Experimentalphysik, Hamburg, Germany
01/06–31/07/2009
Study of Auger processes in gases and at solid surfaces within an attosecond streaking scheme.

Dr. Josef Bartos
Polymer Institute of SAS, Bratislava, Slovakia
15/06–24/07/2009
PALS and polymer dynamics.

Prof. Mario Trioni
CNR, University of Milano-Bicocca, Italy
01–31/07/2009
Electronic and magnetic properties of thin solid film on metals.

Prof. Félix Yndurain Muñoz
Universidad Autónoma de Madrid, Spain
01–31/07/2009
Magnetisem in low dimensional systems.

Prof. Godfrey Gumbs
The City University of New York, USA
13/07–14/08/2009
Plasmons in nanostructures.

Prof. Vladimir Kuznetsov
Tomsk State University, Russia
08/08–08/09/2009
Density functional methods in the theory of phase diagrams of alloys and in the Kondo effects.

Doctorand Stepan Tsirkin
Tomsk State University, Russia
08/08–08/11/2009
Electronic excitations on metal surfaces.

Doctorand Tatiana Menshchikova
Tomsk State University, Russia
08/08–08/11/2009
Excitations on surfaces with defects.

Dr. Alejandro Reyes Coronado
Universidad Nacional Autónoma de México, Mexico
01–30/09/2009
Optical response of resonant metallic nanostructures in surface-enhanced microscopy and spectroscopy.

Prof. Marijan Sunjic
University of Zagreb, Croatia
15/09–30/10/2009
Dynamical response and surface excitations in thin films.

Doctorand Ryan Artuso
National Institute of Standards and Technology, USA
15/10–21/12/2009
Dipolar emission mediated by metalic nanoantennas.

Doctorand Andrey Kuznetsov
Tomsk State University, Russia
11/12–13/01/2010
Magnetic effects on the formation of defects in bulk Fe and in thin Fe films.

Short visits

Prof. Malcolm Stott
Queen's University, Kingston, Canada
31/12/2007–31/01/2008
2D electron gas.

Prof. Godfrey Gumbs
The City University of New York, USA
01/01–30/01/2008
Plasmons in nanostructures.

Prof. Istvan Nagy
Technical University of Budapest, Hungary
07/01–03/02/2008
Various aspects of correlations in extended fermionic systems; spice-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Dr. Alexander Grueneis
Leibniz Institute Dresden, Germany
08/01–11/01/2008
Angle resolved photoemission spectroscopy of carbon systems.

Prof. Thomas Pichler
Leibniz Institute Dresden, Germany
08/01–11/01/2008
High energy spectroscopy of molecular nanostructures.

Dr. Ilya Nechaev
Kostroma State University, Russia
10/01/2007–09/02/2008, 12/01–08/02/2009
Electron excitations in ferromagnetic materials.

Dr. Anibal Iucci
Université de Genève, Switzerland
13/01–20/01/2008, 07/09–04/10/2009
Out of equilibrium Many-Body systems.

Dr. Giuliano Orso
Universite Paris XI, France
13–17/01/2008
Cold gases, disorder low dimensional systems.

Dr. Magnus Paulsson
University of Kalmar, Sweden
15–21/01/2008, 9–22/11/2008, 12–24/01/2009
Inelastic Transport through atomic and molecular wires.

Doctorand Christine Gerstl
Institut für Festkörperforschung, Jülich, Germany
15/01–15/02/2008, 13–24/07/2009
Characterization of the dynamics of polyalkylene-oxides.

Dr. Nicolas Lorente Palacios
Centro de Investigación en Nanociencia y Nanotecnología (CIN2-CSIC), Bellaterra, Spain
15–18/01/2008, 03–04/08/2009
Inelastic Electron Tunnelling Spectroscopy.

Dr. Karlo Penc
Research Institut for Solid State Physics and Optics, Budapest, Hungary
20–29/01/2008
Interacting one dimensional systems.

Prof. Arthur Ernst
Max Planck Institute of Microstructures, Germany
21–24/01/2008, 25–30/05/2009
Magnetism from first principles: a multiple scattering approach.

Dr. Didier Long
Rhodia, Lyon, France
21–22/01/2008
Water in industrial polymers

Dr. Paul Sotta
Rhodia, Lyon France
21–22/01/2008
Water in industrial polymers.

Dr. Ludovic Odoni
Rhodia, Lyon, France
21–22/01/2008
Water in industrial polymers.

Dr. Sampsa Riikonen
Helsinki University of Technology, Finland
25/01–24/02/2008, 14/01–03/02/2009
Theoretical studies of complex surface reconstructions.

Dr. Marius Wanko
Bremen Center for Computational Materials Science, Germany
28/01–01/02/2008
Hybrid methods (QM/M) in biological systems; approaches and spectral tuning of retinal proteins and other chromophores.

Dr. Rainer Hillenbrand
Max Planck Institute, Martinsried, Germany
03–06/02/2008
Scattering-type near-field microscopy for optical/infrared nanoanalytics.

Prof. Mario Trioni
CNR, University of Milano-Bicocca, Italy
10–16/02/2008, 30/11–05/12/2008
Electronic and magnetic properties of thin solid film on metals.

Prof. Amador Menéndez Velazquez
CSIC, Oviedo, Asturias, Spain
10–16/02/2008
Public understanding of science.

Prof. Gustav Bihlmayer
IFF-FZ, Forschungszentrum Jülich, Germany
12–15/02/2008, 02–28/07/2009
Magnetism in low dimensions: Overlayers, wires and atoms.

Dr. Caroline Genix
Université Montpellier II and CNRS Montpellier,France
19–28/02/2008, 10–17/03/2008, 13–19/09/2009
Effect of blending on the dynamics of the system poly(ethylene oxide)/poly(methyl methacrylate).

Prof. Tadaaki Nagao
National Institute of Materials Science, Tsukuba, Japan
20–24/02/2008, 03–06/09/2009
Surface phonons and adlayer crystal structures.

Prof. Concepción Domingo Maroto
Instituto Estructura de la Materia, CSIC, Spain
21–24/02/2008
Visible and infrared molecular spectroscopy.

Dr. Andrew Ho
Imperial College London, United Kingdom
23/02–09/03/2008, 06–12/12/2008, 12–17/09/2009, 08–17/02/2009
Effects of disorder in one-dimensional quantum liquids, and phase diagram of binary mixtures of one-dimensional harmonic fluids.

Dr. Joerg Kroeger
University of Kiel, Germany
28/02–01/03/2008
Electrical conductance of single atoms and molecules.

Prof. Roderic Quirk
The University of Akron, USA
01/03–08/03/2008, 11–19/07/2008, 11–17/01/2009, 18–25/07/2009
Synthesis of functional polymers.

Prof. Emilio Artacho Cortés
University of Cambridge, United Kingdom
09–12/03/2008, 31/08–05/09/2009, 15/07–08/08/2009
Electronic stopping power in insulators. LDA+U, SIC, exact-exchange in DFT calculations.

Prof. Jorge Kohanoff
The Queen's University, Belfast, Northern Ireland, United Kingdom
09–12/03/2008
Simulations of non-adiabatic electron dynamical processes.

Prof. Ivan P. Chernov
Politechnic University of Tomsk, Russia
16–19/03/2008, 25–29/03/2009
Dynamics of hydrogen in metals under external irradiation.

Dr. Margarita Krutyeva
Universität Leipzig, Germany
16–18/03/2008, 28/09–01/10/2008, 12-25/10/2008
Dynamical properties of complex systems.

Prof. Richard Arinero
Université Montpellier 2, France
07–11/04/2008, 15–18/06/2008, 12–25/11/2008, 29–31/03/2009, 07/05/2009
Dielectric spectroscopy at nano-scale by atomic force microscopy (AFM) techniques.

Prof. Domingo Docampo
ETSE Telecomunicación, Vigo, Spain
08–08/04/2008
Scientific policy.

Prof. Philip Hofmann
University of Aarhus Denmark, University of Liverpool, United Kingdom
16–19/04/2008, 17–20/12/2008
Angle-resolved photoemission in High TC superconductors.

Dr. Katharina Franke
Freie Universitat Berlin, Germany
16–18/04/2008
Resonant electron heating and molecular phonon cooling in single C60 junctions.

Prof. Andrey Kazanskiy
University of San Petersburg, Russia
28/04–16/05/2008
Electron dynamics at adsorbates on metals.

Dr. Sara Pagnotta
Roma Tre University, Italy
28/04–05/05/2008
Water in polymers.

Prof. Francisco Guinea López
Instituto Ciencia Materiales de Madrid, CSIC, Spain
01/05–25/05/2008
Condensed matter physics.

Prof. Mark Stockman
Georgia State University, USA
04–11/05/2008
Nanophotonic.

Prof. Branko Gumhalter
University of Zagreb, Croatia
05–09/05/2008, 03–08/07/2009
Ultrafast electron dynamics on metal surfaces.

Prof. Norbert Mueller
Universität Bielefeld, Germany
05–13/05/2008
Electron spectroscopy, attosecond spectroscopy.

Prof. Jan Skov Pedersen
University of Aarhus, Denmark
14–16/05/2008
Small angle x-ray scattering applied to soft condensed matter and biology.

Prof. Annemarie Pucci
University of Heidelberg, Germany
21–26/05/2008
Infrared spectroscopy.

Doctorand Virginie Boucher
University of Lille (ENSCL), France
25–27/05/2008
Dynamical properties at molecular scale in polymeric materials multi-component and/or nano-structured.

Prof. Cayetano López Martinez
CIEMAT and Universidad Autónoma de Madrid, Spain
26/05/2008
Energía y sostenibilidad.

Prof. John Inglesfield
University of Wales Cardiff, United Kingdom
27–31/05/2008
Embedding in photonics and plasmon bands in metallic nanostructures.

Prof. Adam Kaminski
Iowa State University/Ames Laboratory, USA
02–04/06/2008
Fascinating properties of cuprates.

Prof. Rubén Barrera
Instituto de Física, UNAM, Mexico
06/06–03/07/2008, 15–16/10/2009
Use and abuse of the effective refraction index concept in colloidal systems.

Dr. Philippe Zinck
Ecole Nationale Supérieure de Chimie de Lille, France
12–13/06/2008
New polymeric materials synthetized via coordination polymerization: recent examples from our group.

Prof. Peter Toennies
Max Planck Institut für Dynamik und Selbstorganisation, Göttingen, Germany
15–21/06/2008
Helium atom scattering measurements of vibrations on surfaces.

Prof. Jeanpol Vigneron
Facultés Universitaires Notre-Dame de la Paix, Namur, Belgium
17–22/06/2008
Photonic crystals in the natural world preparation of summer school 2009.

Prof. Wolf-Dieter Schneider
Ecole Polytechnique Fédérale de Lausanne, Switzerland
19–22/06/2008
From single magnetic adatoms to two-dimensional Kondo lattices.

Prof. Hans Christian Schneider
Technische Universität Kaiserslautern, Germany
24/06–03/07/2008
Excitations in small clusters.

Prof. Ulrich Hoefer
Philipps-Universität Marburg, Germany
25/06–13/07/2008
Time-resolved two-photon photoemission of Ar/Cu interface states.

Prof. Wolfgang Bacsa
CEMES UPR-CNRS, Université Toulouse, France
26–29/06/2008
Local optical field mapping in the intermediate field for sub-wavelength optical microscopy, compact spectrometers and sensors.

Dr. Josef Bartos
Polymer Institute, SAS, Slovakia
07–17/08/2008
PALS and polymer dynamics.

Dr. Fritz Keilmann
Max Planck Institute of Biochemistry, Germany
10–14/07/2008
Near-field microscopy.

Prof. Honxing Xu
Chinese Academy of Sciences, Beijing, China
12–20/07/2008
Plasmon enhanced spectroscopy.

Prof. Philip Batson
IBM, New York, USA
16–20/07/2008
Electron energy loss spectroscopy and microscopy.

Prof. Vladimir Nazarov
Chonnam National University, Kwanju, Korea
24/07–12/08/2008
Academia Sinica, Taipei, Taiwan
14/09–08/10/2009
Time-dependent density-functional theory of particle-solid interactions.

Dr. Garnet Bryant
NIST, Maryland, USA
26/07–03/08/2008, 30/08–06/09/2009
Optoelectronic properties of quantum dots and quantum wires. Nanophotonics.

Prof. Vladimir Kuznetsov
Tomsk State University, Russia
06/08–05/09/2008
Density functional methods in the theory of phase diagrams of alloys and in the Kondo effects.

Dr. Rafael Pardo
Fundación BBVA, Madrid, Spain
15/08–30/08/2008
Public understanding of science.

Prof. Alberto Galindo
Universidad Complutense de Madrid, Spain
21/08–03/09/2008
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.

Prof. Cesar Proetto
Centro Atómico Bariloche, Argentina
31/08–10/09/2008, 13–30/09/2009
Position-dependent exchange energy and exact-exchange potential for jellium surfaces.

Dr. Remi Busselez
Universite de Rennes, France
03–05/09/2008
Dynamics at atomic and molecular scale in two-component polymeric systems with dynamic asymmetry by quasielastic neutron scattering and fully atomistic molecular dynamics simulations.

Prof. Archie Howie
Cavendish Laboratory, Cambridge, United Kingdom
09–23/09/2008, 09–23/09/2009
Theory of valence electron excitations by fast electrons.

Doctorand Lei Zhang
Huzhou University, Huzhou, China
10–26/09/2008
Computer simulations of complex polymer systems.

Prof. Maria Silvia Gravielle
IAFE, Universidad de Buenos Aires, Argentina
27/09–04/10/2008
Interaction of laser pulses with metallic surfaces.

Dr. Dieter Richter
IFF-FZ, Forschungszentrum Jülich, Germany
28/09–08/10/2008
Polymer dynamics by neutron techniques.

Prof. Luciano Colombo
University of Cagliari and SLACS (INFM-CNR), Italy
30/09–03/10/2008
Growth phenomena in mixed amorphous/crystalline silicon nanosystems.

Dr. Lutz Willner
IFF-FZ, Forschungszentrum Jülich, Germany
05–10/10/2008
Dynamics and kinetics in polymeric micelles.

Dr. Gilberto Teobaldi
University of Liverpool, United Kingdom
28/10–02/11/2008
DFT-modelling of titania (110) and (011) face.

Prof. Sheldon Lee Glashow
Boston University, USA
29–31/10/2008
Does science progress by blind chance or through intelligent design?

Dr. Miguel Angel Gosalvez Ayuso
Helsinki University of Technology/HUT, Finland
16–22/11/2008
Atomistic simulation of propagating fronts: surface processes and MEMS applications.

Prof. Christos Likos
Heinrich Heine Universität, Düsseldorf, Germany
17–19/11/2008
Effective interactions in soft matter systems

Prof. Stephan Roche
Institut de Nanosciences et Cryogénie, CEA, France
19–23/11/2008
Charge Transport in Low Dimensional Carbon based Materials -Carbon Nanotubes & Graphene-.

Prof. Mario Trioni
CNR, University of Milano-Bicocca, Italy
30/11–05/12/2008
Electronic and magnetic properties of thin solid film on metals.

Dr. Guido Fratesi
CNR, University of Milano-Bicocca, Italy
30/11–05/12/2008
Electronic and structural properties of surface systems.

Prof. Rolf Heid
Forschungszentrum Karlsruhe, Germany
08–11/12/2008
Lattice dynamics of adsorbate-covered surfaces from first principles.

Dr. Anke Schmidt
WWU Münster, Germany
10–16/12/2008
Fentoseconds and spin-resolved electron dynamics in magnetic systems.

Prof. Peter Apell
Chalmers University of Technology, Goteborg, Sweden
11–14/12/2008, 21–24/11/2009
Biophysics: from surfaces modes to wound healing.

Prof. John Dobson
Griffith University Technology Centre, Queensland, Australia
15–22/12/2008
Time dependent density functional theory and van der Waals interactions.

Prof. Bo Hellsing
Chalmers and Göteborg University, Sweden
17–20/12/2008, 18–22/05/2009
Electron-phonon interactions on metal surfaces.

Dr. Geethalakshmi K. Rangaswamy
Max Planck Institut für Kohlenforschung, Germany
08–11/01/2009
Theoretical chemistry- Investigation of Biologically active molecules using DFT computed NMR parameters from QM/MM optimized models.

Dr. Sangita Bose
Max Planck Institute for Solid State Reserach, Stuttgart, Germany
22–24/01/2009
STS, measurements of image states in an external electric field.

Prof. Lawrence Glasser
Clarkson University, USA
25–28/01/2009
Mathematical physics applied to condensed matter.

Doctorand Martin Brodeck
IFF-FZ, Forschungszentrum Jülich, Germany
25/01–08/02/2009
Molecular dynamics simulations of polyethylene oxide (PEO) and PEO/PMMA blends.

Dr. Victoria García Sakai
ISIS facility, Chilton, United Kingdom
25–31/01/2009
Quasielastic neutron scattering in soft matter.

Dr. Roque Hidalgo Alvarez
01–05/02/2009

Dr. Juliane Loichen
Goodyear Technical Center, Luxembourg
03–05/02/2009
Nano-dielectric spectroscopy.

Dr. Stephan Westermann
Goodyear Technical Center, Luxembourg
03–05/02/2009
Nano-dielectric spectroscopy

Dr. Andrey Borissov
Université Paris Sud, France
04–28/02/2009
Time-dependent density functional theory and wave packet propagation methods.

Prof. Philippe Roncin
Université Paris Sud, France
11–15/02/2009
Diffraction of fast atoms at surfaces.

Dr. Chantal Valeriani
School of Physics and Astronomy, University of Edinburgh, United Kingdom
15–17/02/2009
Computer simulations of hard sphere systems.

Dr. Eduardo Sanz García
SUPA, School of Physics and Astronomy, University of Edinburgh, United Kingdom
15–17/02/2009
Computer simulations of colloidal gels.

Saadia Ouchiar
University Institute of Technology, Lille, France
21–28/02/2009
Isothermal crystallization kinetics study on aqueous solution of poly(vinyl pyrrolidone) by both dielectric spectroscopy and optical microscopy.

Prof. Leonid Sandratskii
Max Planck Institute, Halle, Germany
22–25/02/2009
First-principles study of the magnetic properties of complex magnetic system; bulk, surfaces, thin films. The properties include ground state properties, magnetic excitations, thermodynamics.

Dr. Leonor Chico Gómez
Instituto de Ciencia de Materiales de Madrid, Spain
23–27/02/2009
Electronic structure calculations in nanotubes.

Dr. Jorge Quintanilla Tizón
ISIS Rutherford-Appleton Laboratory, United Kingdom
04–09/03/2009, 23/05/2009
Pomeranchuk instabilities in fermi liquids.

Prof. Sergio Monturet Caamaño
Universität Potsdam, Potsdam-Golm, Germany
15–28/03/2009
Calculation of disperssive bands: tertrathiafulvalene adsorbed on lead.

Dr. Cedric Lorthioir
Université Paris 12, France
19/03–17/04/2009
Segmental dynamics of polymer chains in POSS-based nanocomposites by solid-state NMR and dielectric spectroscopy.

Dr. Gustavo Catalán Bernabé
University of Cambridge
21–23/03/2009
Electroceramic oxide nanostructures.

Prof. Adnen Mlayah
Université Paul Savatier, Toulouse, France
30–31/03/2009
Plasmon and acoustic phonon coupling.

Prof. Antoine Salin
Université Bordeaux 1, France
30–31/03/2009
Dissociation dynamics of diatronic molecules at metal surfaces. Non-adiabatic effects.

Prof. Philippe Tordjeman
Université Montpellier 2, France
30–31/03/2009
Nanodielectric of polymer.

Dr. Sebastián Bergeret Sbarbaro
Universidad Autónoma de Madrid, Spain
30/03–03/04/2009
Achievements challenges in the field of superconducting nanostructures.

Dr. Sucismita Chutia
Universite Paris-Sud, France
31/03–03/04/2009
Quantum doped with magnetic materials: manganese, iron and nickel.

Dr. Amadeo Lopez Vazquez de Parga
Universidad Autónoma de Madrid, Spain
01–03/04/2009
Scanning tunneling microscopy in ultra high vacuum in molecules deposited in metallic surface. Spatially resolved spectroscopy on graphene.

Dr. Uwe Bovensiepen
Freie Universität Berlin, Germany
05–11/04/2009
Time resolved spectroscopy of surfaces and interfaces.

Prof. Eduard A.B. Koenders
Technische Universiteit Delft, The Netherlands
15–15/04/2009
Microscopic simulations in cement and concrete.

Prof. Luis Oro Giral
Instituto Universitario de Catálisis Homogénea, Universidad de Zaragoza, Spain
16–16/04/2009
Chemistry, environment and sustainability.

Dr. Javier Carretero González
Instituto Ciencia y Tecnologia de Polimeros, CSIC, Spain and The Alan G. MacDiarmid Nanotech Institute, University of Texas at Dallas, USA
20–21/04/2009
Dispersion, interfacial strength and nanoclay mobility relationships in polymer nanocomposites.

Prof. Pedro de Andres Rodriguez
Instituto de Ciencia de Materiales de Madrid, Spain
20–24/04/2009
Adsorption and diffusion of atomic and molecular hydrogen on graphene and graphite.

Prof. Anadi Bhattacharjee
Laboratoire de Physique des solides, Université de Paris Sud, France
22–25/04/2009
Optical properties of quantum dots doped with Mn.

Dr. Vincent Huc
Institut de Chimie Moléculatire et des Matériaux d'Orsay, France
03–05/05/2009
Mixed hybridization systems: beyond the C60

Dr. Thomas Bach
Omicron Nanotechnology
11–15/05/2009
Low frequency noise spectrum in the VT-STM.

Dr. Masud Haque
Max Planck Institute for the Physics of Complex Systems, Germany
19–23/05/2009
Pomeranchuk instabilities in fermi liquids.

Dr. Pawel Buczek
Max Planck Institute of Microstructure Physics, Germany
25–30/05/2009, 02–30/09/2009
Surfaces and thin film magnons.

Dr. Eric Suraud
Université Paul Sabatier, Toulouse, France
27–29/05/2009
Irradiation of clusters and molecules: signals from electrons.

Prof. Javier Tejada Palacios
University of Barcelona, Spain
12–13/06/2009
Magnetic deflagration and detonation.

Prof. Hrvoje Petek
University of Pittsburgh, USA
14–21/06/2009
Electron dynamics in time domain.

Dr. Manfred Matena
University of Basel, Switzerland
14–17/06/2009
Hybrid surface state band in a porous molecular network on Cu(111).

Prof. Marco Bernasconi
Universita di Milano Bicocca, Italy
16–17/06/2009
Ab initio simulation of materials.

Prof. Stefano Ossicini
Universidad de Modena and Reggio Emilia, Italy
23/06–28/06/2009
Photovoltaic materials: nanowires and biostructure.

Dr. Ivo Souza
University of Berkeley, USA
24–27/06/2009
Theory of polarization and orbital magnetization in condensed matter.

Prof. Carlos Jimenez
Universidad de la Coruña, La Coruña, Spain
25–27/06/2009
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Instituto de Matemáticas y Física Fundamental, CSIC, Madrid, Spain
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Ecole Polytechnique Palaiseau, France
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Dr. Silke Biermann
Ecole Polytechnique Paris, France
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Queen's University, Canada.
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Prof. Lukas Novotny
The Institute of Optics, University of Rochester, USA
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Doctorand Simona Achilli
University of Milano-Bicocca, Italy
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Prof. Svetlana Kulkova
Physics and Materials Science, Russian Academy of Sciences, Tomsk, Russia
03–31/07/2009
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Prof. Ian P. Hamilton
Wilfrid Laurier University, Ontario, Canada
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Prof. Jean Marie Lehn
ISIS-Université Louis Pasteur, Strasbourg, France
07–09/07/2009
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Doctorand Jonathan Janoski
The University of Akron, USA
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Dr. Ignacio Iglesias Casarrubios
Universidad de Murcia, Spain
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Dr. Laura Chantada
University of Fribourg, Switzerland
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Dr. Andriy O. Lyakhov
New York Center for Computational Science, State University of New York at Stony Brook, USA
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Prof. José Maria Soler Torroja
Universidad Autónoma de Madrid, Spain
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Dr. Zelia Zanolli
Universite Catholique de Louvain, Belgium
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Dr. Nicolas Lorente Palacios
Centro de Investigación en Nanociencia y Nanotecnología (CIN2-CSIC), Spain
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Prof. Baruh Horovitz
Ben Gurion University, Beer-Sheva, Israel
10–12/08/2009
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Prof. Joachim Krenn
Karl-Franzens-University Graz, Austria
03–07/09/2009
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Dr. Claudio Horowitz
Centro Atómico Bariloche, Argentina
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Dr. Blas Pedro Uberuaga
Los Alamos National Laboratory, USA
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Prof. Daw-Wei Wang
National Tsin Hua University, Taiwan
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Prof. Yutaka Wakayama
National Institute for Materials Science,
Advanced Electronic Materials Center, Tsukuba, Japan
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Prof. Stefan Maier
Imperial College London, United Kingdom
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Dr. José Ignacio Latorre Sentis
Universitat de Barcelona, Spain
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Prof. Vladlen Zhukov
Ural Branch of Russian Academy of Sciences,
Ekaterinbourg, Russia
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Dr. Pablo Gamallo Belmonte
Universidad de Barcelona, Spain
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Prof. Yuri Rakovich
Centre for Research on Adaptive Nanostructures and Nanodevices, Trinity College Dublin, Ireland
15–16/10/2009
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Prof. Matthias Bickelhaupt
Scheikundig Laboratorium der Vrije Universiteit,
Amsterdam, The Netherlands
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Dr. María Blanco Rey
University of Cambridge, United Kingdom
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Prof. Félix Yndurain Muñoz
Universidad Autónoma de Madrid, Spain
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Prof. Gian Paolo Brivio
Universitá di Milano Bicocca, Italy
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Prof. Maciej Kolwas
Institute of Physics, Polish Academy of Sciences, Poland
09–12/11/2009
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Prof. Dudley Herschbach
Harvard University, Massachusetts, USA
12/11/2009
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Dr. Juan Carlos Cuevas
Universidad Autónoma de Madrid, Spain
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Dr. Pauli Virtanen
Helsinki University of Technology, Finland
15–18/11/2009
Microwave control of the supercurrent in hybrid weak links.

Dr. Rubén Esteban Llorente
Institut d'Optique, France
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Dr. Alejandra Sornosa
Instituto de Investigaciones Biomédicas, Spain
17–19/11/2009
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Prof. Raúl Villar Lázaro
Universidad Autónoma de Madrid, Spain
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Prof. Eugene Sherman
Ikerbasque UPV/EHU, Spain
24–24/11/2009
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Dr. Theyencheri Narayanan
European Synchrotron Radiation Facility, France
29–30/11/2009
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Dr. Antonio Politano
Universidad Autónoma de Madrid, Spain
30/11–02/12/2009
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Prof. Hrvoje Petek
University of Pittsburgh, USA
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Alexander Grueneis, Leibniz Institute, Dresden, Germany

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Thomas Pichler, Leibniz Institute, Dresden, Germany

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Arthur Ernst, Max Planck Institute of Microstructures, Halle, Germany

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Karlo Penc, Research Institute for Solid State Physics and Optics, Budapest, Hungary

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Gustav Bihlmayer, IFF-FZ, Forschungszentrum Jülich, Germany

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Mario Trioni, CNR, University of Milano-Bicocca, Italy

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Concepción Domingo Maroto, Instituto Estructura de la Materia del CSIC, Madrid, Spain

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Philip Batson, IBM, New York, United States

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Miguel Angel, Gosalvez Ayuso, Helsinki University of Technology/HUT, Finland

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Andriy O. Lyakhov, New York Center for Computational Science,
State University of New York at Stony Brook, USA

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Tsukuba, Japan

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Yuri Rakovich, Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN)
Trinity College Dublin, Ireland

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MatthiasBickelhaupt, Scheikundig Laboratorium der Vrije Universiteit, Amsterdam, The Netherlands

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María Blanco Rey, University of Cambridge, United Kingdom

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Maciej Kolwas, Institute of Physics of the Polish Academy of Sciences, Poland

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Dudley Herschbach, Texas A&M University, USA

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Raúl Villar, Universidad Autónoma de Madrid, Spain

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Eugene Sherman, Ikerbasque UPV/EHU, Bilbao, Spain

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Antonio Politano, Universidad Autónoma de Madrid, Spain

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Hrvoje Petek, University of Pittsburgh, USA

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First Symposium of the nanoICT Coordination Action

February 26, 2008

ORGANIZERS
Antonio Correia (Fundación Phantoms, Spain)
Daniel Sanchez Portal (CSIC-UPV/EHU, DIPC, Spain)

Nanoelectronics represent a strategic technology considering the wide range of possible applications. These include telecommunications, automotive, multimedia, consumer goods and medical systems. In the semiconductor industry, Complementary Metal Oxide Semiconductor (CMOS) technology will certainly continue to have a predominant market position in the future. However, there are still a number of technological challenges, which have to be tackled if CMOS downscaling should be pursued until feature sizes will reach 10 nm around the year 2015-2020. This miniaturization will offer opportunities for alternative nanodevices (biomolecular-based technologies and nanomechanics) to be incorporated into CMOS platforms providing an increasing diversification of functions.

The EC policies aiming at maintaining Europe at the forefront of the Information Society, through investment in the future key domains or aiming at optimising the development and diffusion of emerging technologies are clearly within the scope of the recently launched nanoICT Coordination Action (CA). High-level dissemination activities within nanoICT CA will help to establish a critical mass of R&D at a European level and to stimulate development of an interdisciplinary community of researchers.

CONTRIBUTIONS

Antonio Correia (Fundación Phantoms, Spain)
nanoICT Coordination Action

Henri Jaffrès (CNRS/Thales, France)
Spin injection in semiconducting nanostructures and heterostructures: issues and perspectives

Marek Szymonski (Jagiellonian University, Poland)
Anchoring and LT-STM/STS characterization of single organic molecules at semiconducting and insulating surfaces

Ricardo Diez-Muiño (CSIC-UPV/EHU, Spain)
Non-adiabatic effects in the reactivity of molecules at metal surfaces

Guillermo Villanueva (EPFL, Switzerland)
MEMS & Nanotechnology

Bill Milne (University of Cambridge, UK)
Carbon Nanotubes- the future of Electronics?

Robert Baptist (CEA-LETI, France)
Nanoscience & Nanoelectronics at CEA

Andres Arnau (DIPC / EHU-UPV, Spain)
Formation of dispersive hybrid bands at an organic-metal interface

Clivia Sotomayor Torres (Tyndall Institute, Ireland & ICN, Spain)
Nanophotonics in the European Research Area: the PhOREMOST perspective

Number of participants: 34

Ultrafast2008

International Symposium

Electron dynamics and electron mediated phenomena at surfaces: femto-chemistry and atto-physics

May 7-8, 2008

ORGANIZERS
Raimundo Pérez-Hernández and Juan A. González-Palomino (Fundación Ramón Areces, Spain)
Pedro M. Echenique and Daniel Sanchez Portal (DIPC, Spain)

The UltraFast2008 workshop was co-organized by the Ramon Areces Foundation and DIPC. The symposium took place at DIPC and gathered a relatively small and selected group of scientists working in the field of electron dynamics and related subjects. The focus was mainly on the implications of the dynamical processes to the basic understanding of the physics and chemistry of materials and, in particular, of surfaces. Some lectures on the state of the art in fast time-dependent processes in atoms and molecules were also included. The aim of this high-level scientific meeting is to debate about the current status of the field, new perspectives and hot topics, and the basic physics underlying observed phenomena. Some important open questions are: Can chemical and biological reactions be steered by controlling electronic motion on molecular orbitals? How does radiation damage biological systems? What are the most effective ways to excite atoms and molecules to highly excited states and how this excitation and the subsequent decay processes can be influenced by electromagnetic fields? Can electromagnetic fields be used to influence the flow of electrons in nanometer scale electronic devices? Will this open a route for a faster operation of electronic devices?

Attophysics and femtochemistry
Attophysics and femtochemistry are the sciences of electrons in motion. Electrons in motion carry electronic current, emit electromagnetic waves, create or destroy molecules, and cause radiation damage in biological systems. Consequently, they are key players in information, industrial, and medical technologies and physical, chemical, and life sciences likewise. In integrated circuits their motion switches current and voltage within picoseconds. In molecules electrons form chemical bonds. On being excited they can trigger chemical and biochemical reactions within femtoseconds. Their oscillatory motion in atoms with a period of 1-2 femtoseconds or less is responsible for emission of visible, ultraviolet, and x-ray light. Electrons travel relevant distances in atoms, molecules, and nanometer-scale semiconductor structures in tens to thousands of attoseconds. Obtaining a detailed in-sight into this motion and gaining the ability to control it will have important implications for many fields of science. Speeding up electronics, steering chemical/biochemical reactions, developing sources of laser-like ultraviolet and x-ray light, and better radiation therapies most likely constitute only a minority of future implications.

CONTRIBUTIONS

Dr. Adrian L. Cavalieri (Max-Planck-Institut für Quantenoptik, Germany)
Attosecond physics

Prof. Dr. Ulrich Heinzmann (Universität Bielefeld, Germany)
Attosecond time-resolved photoemission on metal surfaces

Prof. A. K. Kazansky (V.A. Fock Institute of Physics, Saint-Petersburg State University, Russia)
Some computations for the attosecond streaking experiments

Prof. Dr. Wilfried Wurth (University of Hamburg, Germany)
X-ray spectroscopic methods to study dynamical processes in materials

Prof. Dr. Helmut Zacharias (Physikalisches Institut Westfälische-Wilhelms Universität, Germany)
Electron dynamics at surfaces at high photon energies using the XUV Free Electron Laser (FLASH)

Prof. Dr. Hrvoje Petek (University of Pittsburgh, USA)
Ultrafast photoemission electron microscopy: Imaging light with electrons on femto/nano scale

Prof. Andrey G. Borissov (Université de Paris-Sud, France)
Electron propagation along Cu nanowires on Cu(111) surface

Prof. Branko Gumhalter (Institute of Physics, Zagreb, Croatia)
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Prof. Dr. José Ignacio Pascual (Freie Universität Berlin, Germany)
Electron dynamics at metal surfaces "visualized" with STM

Dr. Jörg Kröger (Christian-Albrechts-Universitaet zu Kiel, Germany)
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Prof. Dr. Hans-Joachim Freund (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)
Structure, morphology and electronics of nanoparticles on oxide surfaces

Prof. Dr. Martin Wolf (Free University Berlin, Germany)
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Prof. Dr. W. Pfeiffer (Universität Bielefeld, Germany)
Spatio-temporal control of nanoptical fields

Prof. Dr. Martin Weinelt (Max Born Institute, Berlin, Germany)
Hot spots and spin waves

Prof. Dr. Thomas Fauster (Universität Erlangen-Nürnberg, Germany)
Scattering of electrons in image-potential states

Prof. Dr. Ulrich Höfer (Philipps-Universität Marburg, Germany)
Dynamics of image-potential resonances

Prof. Dr. Mark I. Stockman (Georgia State University, USA)
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Dr. Tadaaki Nagao (National Institute for Materials Science, Japan)
Atom-scale plasmonics: molding plasmons into atom chains and atoms sheets

Prof. Dr. Dietrich Menzel (TU München, Germany)
Photochemistry at metal nanoparticles

Prof. Dr. W. Eberhardt (BESSY, Berlin, Germany)
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Prof. Dr. Reinhard Doerner (Institut für Kernphysik, Germany)
Ultrafast Probing of Core Hole Localization in Diatomic Molecules

Prof. D. R. Herschbach (Harvard University, USA)
Electron Dynamics in Surface Chemistry

Number of participants: 41

Quantum Coherence and Controllability at the Mesoscale

May 12-23, 2008

ORGANIZING COMMITTEE
Boris L. Alschuler (Columbia University, New York, USA)
Miguel A. Cazalilla (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)
Vladimir I. Falko (Lancaster University, UK)
Francisco Guinea (ICMM-CSIC, Spain)

CONTRIBUTIONS

Carlo Beenakker
Shot noise in graphene

Xavier Waintal
Do metals exits in two dimensions? A study of many-body localization in high mobility Si MOSFETs

Thierry Giamarchi
Low dimensional systems and cold atomic gases

Alejandro Muramatsu
Nonequilibrium dynamics of strongly correlated quantum gases

Mark Raizen
Generation of few-body atomic number states towards scalable entanglement

Fernando Sols
Andreev reflection in bosonic condensates

Gora Slyapnikov
Anderson localization of evolving Bose-Einstein condensates

Natan Andrei
Quantum impurities out of equilibrium

Massimo Inguscio
Anderson localization of ultra-cold atoms in random lattices

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New route to supersolid phases: dipolar interactions in spinor condensates

Ehud Altman
Probing non local order parameters in highly correlated Bose insulators

Oleksiy Kashuba
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Konstantyn Kechedzhi
Magneto-phonon rensonance in graphene

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Adrian Batchtold
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Leonid Glazman
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Alex Kamenev
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Wolfgang Schleich
Gauss sums and factorization of numbers

Yuki Kawaguchi
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Yuval Gefen
Weak Measurements in Solid State

Gerd Schön
Decoherence and Relaxation in Driven Circuit QED systems

Yuri Galperin
Non-Gaussian decoherence in qubits due
to low-frequency noise

Alexander Tartakovskii
Nuclear spin effects in optically pumped semiconductor quantum dots

Enrique Louis
Transport through organic molecules containing magnetic atoms: effects of symmetry and Coulomb interaction

Baruch Horovitz
The dephasing scenario of a particle on a ring with dissipative environments

Nicolas Agrait
Ultralong natural graphene nanoribbons

Maria Vozmediano
Topological disorder, curvature, and minimal conductivity in graphene

Marco Polini
Pseudospintronics with semiconductors and graphene bilayers

Number of participants: 50

1st DIPC-nanoGUNE-ICFO Meeting

May 20, 2008

This meeting is the first encounter between research teams at ICFO, DIPC and nanoGUNE to obtain first hand information about ongoing research projects and explore possible collaborations on specific projects dealing mainly with nanophotonics.

A main topic of research, both at ICFO and DIPC, is related to the study of optical antennas for sensing and enhanced fluorescence. Teams of both institutes gave presentations on this topic and explored possible collaborations for further research on nanoantennas.

CONTRIBUTIONS

P. M. Echenique
Acoustic plasmons

N. Van Hulst
Molecular nanophotonics

J. Aizpurua
Plasmonic nanoantennas

H. Petek
Ultrafast photoemission electron microscopy: Imaging light with electrons on femto/nano scale

G. Badenes
Nanophotonic devices

E. Ortega
Tuning electronic states in self-assembled metallic superlattices

R. Hillenbrand
Near-field nanoscopy

J. Martorell
Non-linear nanophotonics

D. Sanchez Portal
Electronic structure from first principles

R. Quidant
Plasmon nano-optics

T. Pitarke
nanoGUNE: The big challenge of the small

Number of participants: 12

New Frontiers in Magnetism

September 22, 2008

ORGANIZERS
Pepa Cabrera Sanfelix (DIPC, Spain)
Pedro M. Echenique (DIPC and CSIC-UPV/EHU, Spain)

DIPC hosted a meeting of leading researchers in the field of Magnetism. The purpose of this symposium was to acknowledge Professor Agustin Del Moral's contribution to science and celebrate the recent publication of his book *Handbook of Magnetostriction and Magnetostrictive Materials*. The goal of the meeting was to bring together researchers actively working in any field related to magnetism, particularly low dimensional systems, and discuss recent results and the future perspectives.

2008

CONTRIBUTIONS

A. Howie
Time and Frequency - the new Frontiers in Microscopy

F. Yndurain
Magnetism in low dimensional systems

A. Berger
Controlling Granular Magnetic Materials on the Nano-Scale

M. J. Azanza
Magnetic Field Effects on Neurones

D. Sánchez-Portal
Magnetism of graphene substitutionally doped with transition metals

A. Ayuela
Magnetic Induced Shape-Memory Alloys

L. Panina
Adaptive Metamaterials Based on Ferromagnetic Wires

A. Hernando
Microwave attenuation induced by metallic microwires embedded in a dielectric matrix

F. Flores
A new N-fold degenerate model for transition metal single atom Kondo resonances

P. M. Echenique
Electron Dynamics at Surfaces

A. Del Moral
Speech about the book: "Handbook of Magnetostriction And Magnetostrictive Materials"

Number of participants: 14

Workshop on Bio-Inspired Photonic Structures

July 9-15, 2009

ORGANIZING COMMITTEE
Jean-Pol Vigneron (University of Namur, Belgium)
Pedro Miguel Echenique (DIPC and CSIC-UPV/EHU, Spain)
Amand Lucas (University of Namur, Belgium)
Giorgio Benedek, (Università degli Studi di Milano, Italy)
Javier Aizpurua (CSIC-UPV/EHU, Spain)

This meeting, simultaneously a workshop and a summer school, will include tutorials and research seminars on the biological and physical aspects of photonic structures. It was organized in the splendid venue of the San Sebastian historic Miramar Palace. Established researchers and students from physics, chemistry, biology and engineering with a strong interest for interdisciplinary collaboration, were all welcome.

2009

The meeting covered many aspects of biophotonics: quantitative study of nanomorphology, optical properties, biological functions of colors, taxonomic search for species of interest, reverse engineered modelling and computer simulations, bio-mimetic devices, etc. The physical mechanisms involved in these structures are inspiring for device applications in material science and optical engineering.

CONTRIBUTIONS

Andrew Parker Evolution's Big Bang- the Origin of Optics
Eli Yablonovitch Applications of Photonic Crystal Pigments in Technology
Doekele Stavenga Vision and colors
Jacques Livage Pigmentary coloration
Jean-Pol Vigneron Physics of structural coloration
Andrew Parker Evolutionist's point of view
Richard Prum Optics and self assembly of amorphous photonic nanostructures in birds
Jacques Pasteels Animal defense strategies
Jian Zi Biological Photonic Crystal
Jacques Lafait Defining and measuring color
Serge Berthier Multiscale aspects of visual appearance
Michel Milinkovitch Molecular Phylogeny and Evo-Devo
Claus Nielsen Zoological systematics and classification
Cefe López Opal Structures
Gustaaf Van Tendeloo Electron microscopies
László Biró Bio-inspired artificial structures
Davy Galliot Composite organic—Inorganic Butterfly Scales: What Do We learn When Disorder Meets Order!
Claus Helix Nielsen Biomimetic membranes for separation and sensor applications

Number of participants: 66

Summer School on Simulation Approaches to Problems in Molecular and Cellular Biology

August 31 - September 5, 2009

ORGANIZING COMMITTEE

Paolo Carloni (SISSA and INFM DEMOCRITOS, Italy)
Michele Parrinello (ETH Lugano,Switzerland)
Ursula Rothlisberger (EPFL, Switzerland)
Daniel Sanchez Portal (CSIC-UPV/EHU, DIPC, Spain)
Angel Rubio (CSIC-UPV/EHU, Spain)

Cellular functions - like growth, (programmed) cell death, metabolism etc - ultimately depend of interactions between macromolecules encoded by DNA. Proteins and RNA directly control the cell and regulate its functions through the reactions they perform, by allosteric changes driven by endogeneous and exogeneous factors and by their mutual interactions. All of these processes involve molecular recognition, i.e. the process by which two or more biological molecules interact to form a specific complex. Molecular recognition is dominated by short-range, often transient, interactions at the contact surface of the interacting molecules. Even conformational changes and assembly of very large macromolecular aggregates, which can be propagated through long distances (tens of Angstroms), are the sum of local interactions between small molecules (like messengers) or macromolecules with their cellular targets.

Ultimately, therefore, even the understanding of the integration of biological complexes into cellular pathways (the so called 'systems biology') requires mechanistic understanding of the physical basis of molecular recognition. A quantitative description of cellular pathways in molecular terms is still mostly missing, although it would strongly impact on pharmaceutical sciences, as drugs target (and mutations affect) pathways, rather than single biomolecules. Such information is also crucial in nanobiotechnology, e.g. to design artificial sensing devices, which in Nature involve entire cascades of events and not only a single protein.

Molecular simulation constitute a key field to contribute to this issue. It can predict structure, dynamics, energetics, reactivity and spectroscopic properties of the cellular components (i.e. large macromolecular aggregates) involved in these pathways.

Tremendous challenges have to be taken before this ambitious goal can be reached. First, the systems are very complex and so are the interactions involved. In addition, ligand-protein processes involve small changes of free energies (less than 1 eV for non-covalent protein-protein interactions), and they are often entropy-driven. Next, the environment is very complex: cell membranes are far from being a simple lipid bilayer whilst the cytoplasm is far from being a simple aqueous solution. Finally, most often experimental structural information is partially or totally lacking.

Scientific Objectives

The School's main goal is to present recent developments and applications of biomolecular simulation approaches aimed at predicting structure, dynamics and energetics of biomolecules. Aspects of bioinformatics-based structural prediction algorithms will be also presented.
Topics include:
Simulation of rare events
Prediction from first principles of spectroscopic and redox properties of biomolecules
Protein and nucleic acid structure prediction
Critical analysis of the force fields used for biomolecular simulation
Molecular simulation of cellular events
Simulation in molecular medicine

CONTRIBUTIONS

Hutter Juerg (University of Zurich, Switzerland)
Progress in large scale density functional calculations
Calculation of NMR and EPR parameters for proteins in solution

Alber Frank (UCLA, Los Angeles, USA)
Determining the structures of macromolecular assemblies – Part 1
Determining the structures of macromolecular assemblies – Part 2

Voth Gregory A. (University of Utah, Salt Lake City, USA)
Rigorous coarse-graining of condensed phase and biomolecular systems
Multiscale modeling of proteins and membranes: from the molecular to the mesoscale

Cascella Michele (UNIBE, Bern, Switzerland)
Development of unbiased coarse grained potentials for simulations of proteins

Dal Peraro Matteo (EPFL Lausanne, Switzerland)
Coarse-grained electrostatics in multiscale simulations of proteins

Lavery Richard (Institut de Biologie et Chimie des Protéines, Lyon, France)
DNA dynamics and recognition
Coarse-grain models of protein mechanics

Orozco Modesto (Institute for Research in Biomedicine, Barcelona, Spain)
Pushing the boundary of MD simulations. Proteome scale atomistic simulations
Coarse grained dynamics simulations of proteins and nucleic acids

Sulpizi Marialore (University of Cambridge, UK)
Redox properties in metalloproteins
Pka calculations from DFT-based MD simulations

Dal Peraro Matteo (EPFL Lausanne, Switzerland)
Proton conduction and drug binding in the M2 channel from Influenza A virus

Cascella Michele (UNIBE, Bern, Switzerland)
Electronic structure/function relationship in copper-bound redox proteins

Gervasio Francesco (Fundacion CNIO - Carlos III, Madrid, Spain)
Quantitative structure-activity relationship with Metadynamics and Path-collective variables: ligand binding
Quantitative structure-activity relationship with Metadynamics and Path-collective variables: conformational selection and induced fold effects

Piana Stefano (D.E. Shaw Research, New York, USA)
The precision and accuracy problems in MD simulations
Improving force fields for MD simulations

Rubio Angel (ETSF, Donostia-San Sebastian, Spain)
First principles description of the optical properties of biochromophores

Tavernelli Ivano (EPFL, Lausanne, Switzerland)
TDDFT as a tool in chemistry and biology
Light driven reactions in biological systems

Rovira Carme (ICREA, Barcelona, Spain)
Substrate conformational changes in glycoside hydrolase catalysis
The reaction mechanisms of heme peroxidases by QM/MM simulations

Grubmüller Helmut (MPI, Gottingen, Germany)
Conformational motions of biological macromolecules
Molecular dynamics simulations of biological nanomachines: may the force be with you

Raugei Simone (SISSA and INFM-DEMOCRITOS, Trieste, Italy)
Computational vibrational spectroscopy for biomolecules: basics
Computational vibrational spectroscopy for biomolecules: an application to the bacterial resistance to antibiotics

Guidoni Leonardo (Università degli Studi dell'Aquila, L'Aquila, Italy)
Computing vibrational spectra of biomolecules by Quantum Mechanics/ Molecular Mechanics simulations
First principles calculations of photoreceptors

Participant Talks
Brunk Elizabeth (EPFL, Lausanne, Switzerland)
Zhu Lihze (University of Amsterdam, Amsterdam, The Netherlands)
Valeria Losasso (SISSA, Trieste, Italy)
Tipmanee Varomyalin (University of Cambridge, Cambridge, UK)
Deplazes Evelyne (University of Western Australia, Crawley, Australia)
Delemotte Lucie (Université Henri Poincaré, Nancy, France)

Number of participants: 48

Workshop on Inorganic Nanotubes Experiment and Theory

September 2-4, 2009

ORGANIZING COMMITTEE
Andrés Ayuela (CSIC-UPV/EHU, Spain)
Pedro Miguel Echenique (DIPC and CSIC-UPV/EHU, Spain)
Gotthard Seifert (TU Dresden, Germany)
Jorge Sanchez-Dolado (NANOC–LABEIN Technological Center, Bilbao, Spain)

Nanotubes have attracted much attention of experimentalists and theorists. The informations about construction, synthesis and properties of the carbon nanotubes were published in numerous publications and books. At present, not only these new allotropes of carbon focus on fundamental research, but they find also its way in many applications.

Simultaneously with the discovery of the carbon nanotubes a question appeared — Can nanotubular structures be produced only based on carbon? The synthesis of the noncarbon nanotubes was realized in 1992 based on the molybdenum and tungsten disulphides. The hollow 1D nanostructures are not the exclusive phenomena for carbon, but they are possible for other compounds such as MoS2 and WS2! During last 15 years the nanotubes of almost a dozen of inorganic compounds were discovered. Although the inorganic nanotubes were observed soon, one year after the carbon nanotubes, a systematic view on their synthesis, their properties and their potentials for applications is still very limited.

This workshop aimed to provide a forum for communication amongst scientists working in the field of Inorganic Nanotubes. Similar to the vast development on Carbon Nanotubes we hope to encourage the generation of new ideas for the development of novel nanotubular systems and their properties bringing together scientists working both experimentally and theoretically on Inorganic Nanotubes. The frame of the workshop was planned to be small to provide a productive scientific enviroment for interesting and exciting ideas.

The range of topics was rather broad and considered experimental as well as theoretical aspects on:
Synthesis
Structure and Characterization
Mechanical Properties
Electronic and Optical Properties
Applications (tribological, catalysis, solar cells, etc.).

There was also a celebration for the 65th birthday of Prof. Reshf Tenne, who, since the discovery of inorganic nanotubes, has provided significant contributions and strongly influenced this field.

CONTRIBUTIONS

Reshef Tenne
Update on selected topics related to inorganic nanotubes

Alexander Quandt
Boron nanotubes- Theory, experiments, and applications

Julio A. Alonso
Theoretical study of Boron and BeB2 nanotubes

Janice L. Musfeldt
Dynamical charge and structural strain in MoS2 and MnO nanoparticles

Nabeen K. Shresta
Physic self organized TiO2 nanotubes. Formation, properties and applications

Angel Rubio
Excited state properties of BN nanotubes optical and energy loss spectroscopies

Wolfgang Tremel
Synthetic Approaches to Functionalized Chalcogenide Nanotubes

Daniel Kohler
Double-walled bismuth-nanotubes from a chemical top-down — bottom-up approach

Jose I. Martinez
Stability and electronic properties of TiO2 nanostructures with and whituouth B and N doping,

Francesco Mercuri
Polymorphism at the nanoscale and electronic properties of inorganic nanotubes:
A theoretical approach

Mark Wilson
The growth and structure of inorganic nanotubes

Sampsa Riikonen
Computational study of BNNT catalityc synthesis

Dominik Eder
Nanoengineering with residual Catalyst from CNT templates

David Tománek
Studying local properties of MoxSylz nanostructures:From stability to electronic and vibrational structure

Gothard Seifert
The Influence of Defects in Inorganic Nanotubes on Electronic and Mechanical Properties

Andrey Enyashin
Structure and stability of Aluminosilicate Nanotubes

Agnieskza Kuc
Shielding Nanotubes and wires with Imogolite: A route to create nanocables

Hegoi Manzano
Structure and stability in Nanotubes of Cementitious Materials

Number of participants: 30

Atom by Atom:
NANO2009–Perspectives in nanoscience and nanotechnology

September 28-30, 2009

CHAIRMEN
Pedro M. Echenique (DIPC and CSIC-UPV/EHU, Spain)
Jose M. Pitarke (CIC nanoGUNE, Spain)

ORGANIZING COMMITTEE
Andreas Berger
Alexander Bittner
Rainer Hillenbrand
Luis Hueso
Igor Nabiev
Jose M. Pitarke
Daniel Sanchez-Portal

The "NANO2009 – Perspectives in Nanoscience and Nanotechnology" workshop is part of the Atom by Atom conference. NANO2009 followed the successful 'NANO2006 – Perspectives in Nanoscience and Nanotechnology' workshop celebrated in September of 2006 in Donostia-San Sebastian, Basque Country (Spain). It was a multidisciplinary workshop that reviewed the state of the art in the fields of nanomagnetism, nanooptics, self-assembly, nanobiotechnology, nanodevices, and theory and simulation at the nanoscale. NANO2009 fostered discussion on emerging applications with potentially significant impact for the materials, electronic, photonics, and life-science industries, and debate about the current strategy and perspectives in Nanoscience and Nanotechnology.

CONTRIBUTIONS

Emilio Artacho (Cambridge, UK)
Theoretical simulation of nanostructures: from oxide superlattices to topological defects in ferroelectric nanowires

Stephan Roche (Grenoble, France)
Mesoscopic transport in chemically modified forms of carbon based low-dimensional structures

Niek F. van Hulst (Barcelona, Spain)
Nanoscale control of single photon emitters by optical nano-antennas and tailored fs pulses

Stefan Maier (London, UK)
Coherent processes in plasmonic panocavities

Luis Martín-Moreno (Zaragoza, Spain)
Surface waves radiated by a subwavelength aperture in a metal film

Jean-Philippe Bourgoin (Gif-sur-Yvette, France)
Issues related to self-assembly in the context of nanoelectronics

Christina Wege (Stuttgart, Germany)
Nanoshaping with natural precision: self-assembled plant-viral templates as a novel scaffold toolkit

Alexander Govorov (Ohio, USA)
Energy transfer in bio-inspired nanostructures

Stefan Haacke (Strasbourg, France)
Ultrafast bio-molecular dynamics at the nanoscale

Sebastian Mackowski (Torun, Poland)
Controlling absorption of light-harvesting complexes via plasmonic interactions

Gernot Güntherodt (Aachen, Germany)
Spin currents in nanostructures

C. Leighton (Minnesota, USA)
Magnetic phase separation at complex oxide interfaces

Josep Nogués (Barcelona, Spain)
Exchange bias and proximity effects in
'inverted' antiferromagnetic/ferrrimagnetic core/shell nanoparticles

Klaus Ensslin (Zurich, Switzerland)
Electrons in nanostructures — one by one

George Malliaras (Saint Etienne, France)
Organic bioelectronics

Number of participants: 711

BNC Tubes STREP Meeting

October 5-6, 2009

ORGANIZER
Sampsa Riikonen (TKK, Finland)

CONTRIBUTIONS

Theoretical Studies on BNC Nanotubes and Their Synthesis

S. Riikonen
BN bond Stabilization on Iron and Magnesium

G. Lanzani
CN, CC and NN association reactions on a small nanosized cluster

L. Henrard
STM and Electronic Transport Fingerprints of B- and N-Doped Nanotubes

Synthesis of BNC Nanotubes

R. Fleurier
Sorting by density gradient ultracentrifugation of nanotubes

J. Lagoute
Measure od the electronic structure of SWNTs by STM

A. Nasibulin
Mechanistic Investigations of Single-Walled CNT Growth

T. Susi
N-doped SWCNT tube synthesis

J. Beausoleil
Synthesis of MWNT Doped with Nitrogen by FB-CVD

Characterization of BNC Nanotubes

E. Obratsova
Optical and low-field electron emission applications of nanotubes

A. Chernov
Separation on metallic and semiconducting fractions and characterization of single-wall carbon nanotubes

A. Koos
BNC tubes: synthesis and applications

Number of participants: 16

Jülich Centre for Neutron Science Workshop 2009
Trends and Perspectives in Neutron Scattering on Soft Matter

October 5-8, 2009

This international workshop was organized to discuss current status and future trends and possibilities of neutron scattering methods in studying structure and dynamics of soft matter systems. Due to the unique properties of neutrons investigations to reveal structure and dynamics of polymers, colloids, polymer interfaces, composite polymer materials, bio-compatible and bio-mimetic structures, polymer glasses and polymer nanostructures have delivered significant insight into soft matter physics and soft matter molecular structure. Novel dedicated methods as neutron spin echo spectroscopy or time resolved small angle neutron scattering have delivered unique insight into the understanding of soft matter structures and molecules. Recent advancements and future trends in soft matter science and their demands on neutron instrumentation were discussed.

CONTRIBUTIONS

Slow Dynamics

Arantxa Arbe (UPV/EHU, Spain)
Nano-confinement through self-assembly in homopolymers with long alkyl sidegroups: Observation of anomalous relaxation

Christina Alba Simonesco (LLB Saclay, France)
Molecular weight dependence of the viscous slowing down and the glass properties of polymers

Michael Monkenbusch (Forschungszentrum Jülich, Germany)
Neutron Spin-Echo in Soft Matter and Biology, results from and challenges for the instrumentation

Jeremy C. Smith (Oak Ridge National Laboratory, USA)
Dynamics of Biomolecules

Hideki Seto (High Energy Accelerator Research Organization, Japan)
Multi-lamellar structure induced by hydrophilic and hydrophobic ions in a mixture of water and organic solvent

Thomas Hellweg (University of Bayreuth, Germany)
Responsive Microgels in the Presence of Different Counterions: The Hofmeister Effect

Kinetics

Reidar Lund (DIPC, Spain)
Fast Kinetic Processes in Micellar Systems Resolved by Small Angle Scattering

Stefan Egelhaaf (University of Düsseldorf, Germany)
Kinetics of structural transitions in surfactant solutions

Wim Pyckhout-Hintzen (FZ Jülich, Germany)
Molecular Rheology and Quenched Small Angle Scattering in Non-Linear Deformation

Instrumentation

Satoshi Koizumi (Japan Atomic Energy Research Institute, Japan)
Advanced Technique of Ultra-Small-Angle Neutron Scattering Explores a New Scientific Field of Neutron Cell Biology, Covering from a Single Molecule to Cell

Self Assembly

Mitsuhiro Shibayama (University of Tokyo, Japan)
Kinetics, structure, and dynamics of multi-arm poly(ethylene glycol) gels

Thomas Sottmann (University of Cologne, Germany)
Self-assembly in mixtures of water and super-critical CO2

Tim Salditt (Universität Göttingen, Germany)
Structure and Dynamics of Lipid Membranes by Inelastic Neutron Scattering and X-ray Imaging

Nano Composites

Jean-Marc Zanotti (LLB Saclay, France)
Polymer dynamics under quasi-uniaxial confinement. The case of PEO in porous alumina

João Cabral (Imperial College London, United Kingdom)
Phase transitions in polymer-nanoparticle composites

Peter Schurtenberger (University of Fribourg, Switzerland)
Analyzing self-assembled protein clusters, gels and glasses using SANS and neutron spin-echo experiments

Synergies by Combination of Techniques

Peter Müller-Buschbaum (Technische Universität München, Germany)
Lateral structures at buried interfaces as probed with GISANS

Tiberio Ezquerra (CSIC-IEM, Spain)
Probing Ordering Processes in Soft Condensed Matter by using Time Resolved Techniques: from Neutrons to Photons

Michael Haertlein (Institut Laue Langevin, France)
Deuterium labeling of biological macromolecules at the ILL-EMBL Deuteration Laboratory, a platform of the Partnership for Structural Biology (PSB) Programme and its importance for Neutron Scattering studies in biology

Tom McLeish (Durham University, United Kingdom)
Neutron Flow-Mapping and Multiscale Modelling of Controlled-Architecture Polymer Melts

Number of participants: 22

nanoICT School 2009
NanoPhotonics NanoOptics Modelling

October 26-30, 2009

ORGANIZERS
Dr. Antonio Correia (Fundación Phantoms, Spain)
Dr. Daniel Sanchez Portal (CSIC-UPV/EHU, DIPC, Spain)
Dr. Igor Campillo (CIC nanoGUNE, NanoBasque, Spain)

Nanoelectronics represent a strategic technology considering the wide range of possible applications. Many of the potential emerging nanoelectronic applications still require substantial work in order to be transformed into marketable technology. A concerted effort must therefore be made at the European level to both understand and commercialise molecular and atomic scale technology in order to maintain a competitive advantage for Europe and keep Europe at the forefront of the next nanoelectronics revolution, a revolution beyond nanotechnology.

In order for the field of emerging nanoelectronics to continue growing exponentially worldwide and therefore lead to new commercial applications and to change the micro and nanoelectronics paradigm, it is necessary to educate new researchers who can work across traditional disciplines. The EU funded nanoICT project (nº 216165) will establish a broad array of specialised training activities to provide mainly students with interdisciplinary competences in Nanotechnology and more specifically "nano-scale ICT devices & systems" (Emerging Nanoelectronics). These initiatives will generate a new generation of high-skilled interdisciplinary scientists, indispensable to the sustainability of European excellence in the topic considered, but also educate the current working force. The main training event will be a one post-graduate winter school on "ICT nanoscale devices" research domains organized in collaboration with the Donostia International Physics Center (DIPC), CSIC and nanoGUNE.

2009

CONTRIBUTIONS

School 1: NanoOptics and NanoPhotonics
Rainer Hillenbrand (CIC nanoGUNE, Spain)
Juan Jose Saenz (UAM, Spain)
Remi Carminati (ESPCI, France)

nanoICT symposium
Javier Aizpurua (CSIC-UPV/EHU, DIPC, Spain)

School 2: nanoICT modeling issues
Uzi Landman (Georgia Tech, USA)
Stephan Roche (CEA-INAC, France)
Javier Aizpurua (DIPC, Spain)
Daniel Sanchez-Portal (CSIC-UPV/EHU, DIPC, Spain)

Number of participants: 127

5th Laser Ceramics Symposium:
International Symposium on Transparent Ceramics for Photonic Applications

December 9-11, 2009

ORGANIZING COMMITTEE
Chairman
J. Fernandez (UPV/EHU, Spain)
Co-chairs and Promoters
A.A. Kaminskii (Institute of Crystallography, Russian Academy of Sciences, Russia)
K. Ueda (Institute for Laser Science, University of Electro-Communications, Japan)
W. Strek (Institute of Low Temperature and Structure Research, Poland Academy of Sciences, Poland)

5th Laser Ceramics Symposium (LCS): International Symposium on Transparent Ceramics for Photonic Applications is a successive one just after the previous editions in Poland (2005), Japan (2006), France (2007), and China (2008). The aim of this Symposium is to provide a forum for material scientists, chemists and physicists to debate about the state of the art and the perspectives of nanocrystalline ceramics for photonic applications. It would also give to the participants an insight on future advances and research possibilities in these fields and an opportunity for starting fruitful collaborations. The following topics were explored:
Synthesis of optical transparent ceramics
Oxide and non-oxide laser ceramics
Characterization of physical properties
Optical spectroscopy
Composite structure
Ceramic lasers and amplifiers
Ultrashort pulse generation
Applications of optical ceramics
Novel materials and novel fabrication methods

2009

PROGRAM COMMITTEE
Co-chairs
R. Balda (UPV/EHU, Spain)
D. Jaque (Universidad Autónoma de Madrid, Spain)
Members
S. Wang (Shanghai Institute of Ceramics, Chinese Academy of Sciences, China)
G. I. Messing (Penn State University, USA)
T. Taira (Laser Research Center for Molecular Science, Institute for Molecular Science, Japan)
V. B. Kravchenko (FIRE, Russian Academy of Sciences, Russia)
M. Mortier (Ecole Nationale Supérieure de Chimie de Paris, France)
U. Kynast (University of Applied Sciences, Germany)
S. Rand (University of Michigan, USA)

INTERNATIONAL ADVISORY COMMITTEE
Q. H. Lou (Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China)
A. Ikesue (Japan Fine Ceramics Center, Japan)
T. Soules (Lawrence Livermore Laboratory, USA)
D.Y. Tang (School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore)
S.N. Bagayev (Institute of Laser Physics, Russian Academy of Sciences, Russia)
J.L. Adam (University of Rennes, France)

H. J. Kong (Laser Science Research Lab, Korea Advanced Institute of Science and Technology, Korea)
W. Lojkowski (Institute of High Pressure Physics, Polish Academy of Sciences, Poland)
A. Krell (Fraunhofer Institute for Ceramic Technologies and Systems (IKTS), Germany)
R. Chaim (Department of Materials Engineering, Israel Institute of Technology, Israel)
V. Lupei (National Institute for Lasers, Romanian Academy of Sciences, Romania)
Luís Carlos (University of Aveiro, Portugal)

CORRESPONDING ADVISERS OF COMMITTEES
H. Yagi (Konoshima Chemical Co., Japan)
G. J. Quarles (VLOC Incorporated, Subsidiary of II-VI Incorporated, USA)
T. T. Basiev (Institute of General Physics, Russian Academy of Sciences, Russia)
G. Boulon (Claude Bernard-Lyon 1 University, France)
M. Bettinelli (University of Verona, Italy

NATIONAL ADVISORY COMMITTEE
V. Orera (Instituto de Ciencia de Materiales de Aragón, Zaragoza)
D. Levy (Instituto de Ciencia de Materiales de Madrid)
F. Díaz (Universidad Rovira i Virgili, Tarragona)
L.Roso (Universidad de Salamanca)
J. García-Solé (Universidad Autónoma de Madrid)
V. D. Rodríguez (Universidad de la Laguna, Tenerife)
C. Cascales (Instituto de Ciencia de Materiales de Madrid)
L. E. Bausá (Universidad Autónoma de Madrid)
I. Martín (Universidad de la Laguna, Tenerife)

LOCAL ORGANIZING COMMITTEE
J. Fernández (UPV/EHU) *Chair*
R. Balda (UPV/EHU) *Co-chair*
D. Jaque (Universidad Autónoma de Madrid) *Co-chair*
I. Iparraguirre, *Scientific Secretariat*
J. Azkargorta, *Scientific Secretariat*
S. García-Revilla, *Scientific Secretariat*
M.I. Arriortua (UPV/EHU)
T. Rojo (UPV/EHU)
A.J. Garcia-Adeva (UPV/EHU)

SPEAKERS (in alphabetical order)
Dariusz Hreniak (Institute of Low Temperature and Structure Research, Polish Academy of Sciences)
Ulrich Kynast (University of Applied Sciences Muenster, Germany)
Tomonori Matsushita (Laser Research Center for Molecular Science, Institute for Molecular Science, Japan)
Michel Mortier (LCMCP, CNRS - Chimie ParisTech, France)
Gregory James Quarles (VLOC Incorporated, a subsidiary of II-VI Incorporated, USA)
Jasbinder S. Sanghera (US Naval Research Laboratory, USA)
Akira Shirakawa (Institute for Laser Science, University of Electro-Communications, Japan)
Ken Ichi Ueda (Institute for Laser Science, University of Electro-Communications, Japan)
Hideki Yagi (Takuma Works, Konoshima Chemical Co., Ltd. Japan)

Number of participants: 55