DONOSTIA INTERNATIONAL PHYSICS CENTER

2004/05

The cover image depicts a portion of Richard Feynman's 1959 talk, "There's Plenty of Room at the Bottom". This famous speech helped to inspire nanotechnology.

The image was created by Seunghun Hong using dip-pen nanolithography, each letter is one molecule high and made of 16-mercaptohexadecanoic acid.

The width of the speech is 30 microns; which means that over one thousand copies could fit on the head of a pin.

CREDITS

2004/05

Creative direction and design by **Lauren Hammond** (lhammond@wanadoo.fr)
Cover image created under the direction of **Chad A. Mirkin** at the Institute of Nanotechnology, Northwestern University
Opening image by **Carl Pendle**, Photonica
Photography by **Adrian Collins** (www.adriancollinsphotography.co.uk), photograph on page 7 by **Lamia** (Irún, Spain)
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INSIDE Reporting on 2004/05

WELCOME
TO THE DIPC FOUNDATION

Continuing to promote and facilitate the development of basic and oriented research in materials science.

Donostia International Physics Center (DIPC) Foundation was created in 1999, as a fruit of foresighted collaborations between the Departments of Education and Industry of the Basque Government, the University of the Basque Country, the Provincial Authority of Gipuzkoa, the Town Hall of San Sebastian and the savings bank, Kutxa of San Sebastian and Gipuzkoa.

DIPC started as an intellectual center with the principal aim of promoting and facilitating the development of basic and oriented research in materials science to the highest level. DIPC has therefore been open and associated to the University of the Basque Country and an internationalization platform for basic science in the Basque Country in the field of materials science.

In order to meet these goals, in the first consolidation stage, three basic programs were established:

1. Visiting Researchers Program
2. International Workshops Program
3. General Science Communication Program

The aim of the **Visiting Researchers Program** was to attract the best scientists in the field of materials science. Thus, an interaction platform between researchers of high recognition from other countries and our researchers was established. From this platform, the emergence of new joint project proposals would not only be favored but the creation of an international network which allows for a better understanding and diffusion of our own scientific activity.

We will strengthen our future scientific capabilities by building synergies and partnerships with other centers and institutions of our environment.

The **International Workshops Program** was intended to create new platforms for debate in which experts from different arenas but with common goals would contribute to the resolution of hot topics. Rather than adopting the conventional format of a conference, informal meeting with a reduced number of invited scientists was preferred in order to provide plenty of free time for discussions.

Finally, the **General Science Communication Program** was intended to bring the world of science to the public. The social implication of this program is evident at a time when science and technology play a crucial role for the future of our world.

After six years, we can say that the objectives we set from the start have been accomplished. In this period, DIPC has become a center of reference in basic research of **Materials Physics**. The relevance is supported by the quality of the researchers who have visited the center, the international level of the workshops held and most of all, the importance of the scientific contributions derived from the research activity. For instance, during the period of the time of this report, 2004/05, 235 original papers have been published in journals such as, *Physical Review Letters* (26 papers) and *Physical Review* (67 papers). This means that the contribution in 2004/05 from DIPC in these journals is in the order of 7% of the total contribution by Spanish institutions. This is quite an achievement for such a young institution.

It is also important to note the launching of the **Fellows Guipuzkoa**. This program, under the financial support of the Provincial Authority of Guipuzkoa, allows young scientists, mostly from the Basque Country, who have been working abroad, to return. DIPC acts as a "landing platform" by means of a five-year contract.

Along the same line of development, we can include the creation of our in-house Computation Center. The first phase of this center was inaugurated in July 2003 with the aim of becoming an international reference in complex computational physics and materials simulation. After about three years, our Computation Center is approaching its equilibrium stage of operation. We hope that the center will become one of the basic pillars for future developments of scientific activity at DIPC through continuous updates in hardware.

In addition to DIPC's scientific level, it is also gained recognition internationally as a center of innovation, as other universities and research centers have recently shown interest in our model of operation.

Juan Colmenero de León
General Director

Pedro Miguel Echenique Landiribar
President

Alberto López Basaguren
Secretary

Spurred by these remarkable results, we now face the challenge of developing DIPC into a powerful center for basic research and to strengthen our capabilities. The main goal for the near future is the creation of a critical mass of staff researchers at DIPC. The idea does not consist of repeating the schemes of other centers, with permanent staff positions, but of habilitating medium term contract staff (one to three years) in numbers which would allow for the proper exploitation of existing know-how and resources. In order to reach this objective, over last two years we have developed a postdoctoral and PhD contract grant program. These new programs, along with the established Fellows Guipuzkoa, and the external grant systems, will enable for the attainment of a critical mass of researchers based at DIPC. New spaces must be made available, which will involve the refurbishment of the fourth building at the DIPC premises.

Moreover, we will strengthen our future scientific capabilities by building synergies and partnerships with other centers and institutions of our environment. In particular with the Materials Physics Department of the University of the Basque Country, the Materials Physics Institute (joint center of the University of the Basque Country (UPV/EHU) and the Spanish Research Council (CSIC)) and the recently created Nanogune network. We believe this is the route to maintain our ranking on the European and international scene.

Last but not least, we plan to continue publicizing the latest scientific developments and giving young people a taste for science in the framework of our General Science Communication Program. A successful example was the conference organized around Albert Einstein's work and personality in September of 2005, where six Nobel laureates shared the passion for research with over 750 attendants. ■

Basque Government
Department of Industry, Commerce and Tourism
Department of Education, Universities and Research

Eusko Jaurlaritza
Industria, Merkataritza eta Turismo Saila
Hezkuntza, Unibertsitate eta Ikerketa Saila

Gobierno Vasco
Departamento de Industria, Comercio y Turismo
Departamento de Educación, Universidades e Investigación

University of the Basque Country
Euskal Herriko Unibertsitatea
Universidad del País Vasco

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GLOBAL APPEAL
IN SAN SEBASTIAN

DIPC assembles internationally renowned figures to celebrate 100 years since Albert Einstein's annus mirabilis.

On September 5th, 2005, the city of Donostia-San Sebastian hosted an extraordinary gathering to celebrate the centenary of one of the years which marked the 20th century, as well as the history of humankind: the *annus mirabilis* of Albert Einstein. Under the auspices of DIPC, over 750 attendants from the world over, and some 2000 following the event online, shared the experience and insight of six Nobel laureates, and thirteen other leading experts on the figure of Einstein and the impact of his work on modern physics and philosophy.

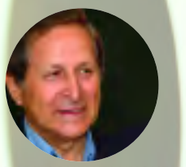
The program, which was aimed at an educated but non specialist audience, attracted public from all age, social and professional groups, dispelling any doubts over the interest of citizens for the intellectual adventure of science, and its repercussions in modern life. Moreover, six months after the event, the number of visits to the official conference website to view the various contributions exceeded 100,000.

The event, which was inaugurated by the Basque President, Juan José Ibarretxe, was followed by a keynote lecture by Nobel laureate Claude Cohen-Tannoudji who elaborated on the subject of Bose-Einstein condensates. Other notable contributions by Nobel laureates Sheldon Lee Glashow, Dudley Herschbach, Antony Hewish, Jean-Marie Lehn and Heinrich Rohrer, were accompanied by outstanding speeches by Ignacio Cirac, Fernando Flores, Alberto Galindo, Gerald Holton, Amand Lucas, Arthur Miller, Pedro Pascual, Rafael Rebolo, José Manuel Sanchez Ron, John Stachel, Clifford Will, Francisco Yndurain and Anton Zeilinger.

The scientific program was accompanied by a social and cultural complement including a concert with Einstein's favorite pieces, cultural visits, and a session of Basque verse making, which revealed some of the special features associated with the Basque Country.

The four day conference resulted in the union of all participants in the enthusiastic appreciation for science as a supreme human endeavor.

The organizing committee wishes to express their thanks to all those who took part in the success of the event, with a special mention to the patrons of DIPC who made the celebration possible. ■



CLAUDE COHEN-TANNOUDJI

Bose Einstein Condensates: A New Form of Matter

JEAN-MARIE LEHN

Steps Towards Complex Matter

ANTONY HEWISH

Pulsar Physics and Testing Einstein

DUDLEY HERSCHBACH

Brownian Motion and Molecular Motors

HEINRICH ROHRER

Nano is Different

SHELDON LEE GLASHOW

What is a Unified Theory?

The conference proceedings, including those of the Nobel laureate speakers, are currently available in dvd format on request from DIPC.

Albert **Einstein** Annus Mirabilis **2005**

SEPTEMBER 5-8, 2005

Chairmen
Prof. A. Galindo (Universidad Complutense, Madrid, Spain)
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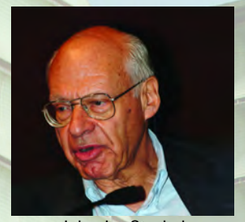
Prof. J.J. Iruin (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)

CONTRIBUTIONS

I. Cirac	**Quantum Information Theory: Challenges and Perspectives**
C. Cohen-Tannoudji	**Bose Einstein Condensates: A New Form of Matter**
F. Flores	**Matter and Form**
A. Galindo	**Einstein and time**
S.L. Glashow	**What is a Unified Theory?**
D. Herschbach	**Brownian Motion and Molecular Motors**
A. Hewish	**Pulsar Physics and Testing Einstein**
G. Holton	**Einstein: Who he thought he was, and why he is still so alive today**
J.-M. Lehn	**Steps Towards Complex Matter: Information, Self Organization and Adaptation in Chemical Systems**
A.A. Lucas	**Einstein and Diffusion Phenomena that Changed the Course of Human Affairs**
A.I. Miller	**Einstein, Picasso: Space, Time and the Beauty that Causes Havoc**
P. Pascual	**Einstein and the Light Quanta**
R. Rebolo Lopez	**Origin and Evolution of the Universe: The Challenges of Cosmology**
H. Rohrer	**Nano is Different**
J.M. Sanchez Ron	**Einstein and Philosophy in the 20th Century**
J.J. Stachel	**Einstein's Greatest Dream —A Background— Independent Physics**
C.M. Will	**Was Einstein Right? The Confrontation between General Relativity and Experiment**
F.J. Yndurain	**Relativity, Photons and Particles**
A. Zeilinger	**Einstein and the Quantum World Today**

The President of the Basque Country, Juan José Ibarretxe (center right) opened the sessions. The keynote lecture was given by Claude Cohen-Tannoudji (fourth from left) and a Welcoming Reception followed in the foyer of Kursaal Auditorium.



John Jay Stachel

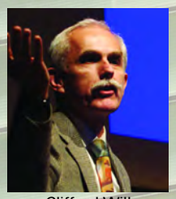
Rafael Rebolo Lopez

The speakers gather outside Hotel Londres: (back row) Profs. Rohrer, Lucas, Miller, Glashow, Yndurain, Herschbach, Zeilinger and Flores, and (front row) Profs. Holton, Hewish, Cohen-Tannoudji, Stachel, Cirac, Pascual and Rebolo.

Anton Zeilinger

Amand Lucas greets Andoni Luis Aduriz

Pedro Echenique with Henrich Rohrer



Clifford Will

Gerald Holton accompanied by his wife, Nina

Unai Ugalde presents Sheldon Lee Glashow

Arantxa Arbe and Juan Colmenero

Pedro Echenique with Antony and Georgene Hewish

Juan José Iruin

Arthur I. Miller

Pedro Pascual with Ignacio Cirac and José María Fernández de Labastida

Alberto Galindo opens the conference with President Ibarretxe

Dudley Herschbach and Francisco José Yndurain

RESEARCH ACTIVITIES

DIPC is dedicated to two main areas of research.

Condensed Matter Physics

Research at the Condensed Matter Physics group is currently focused into the structural, electronic and optical properties of solids, surfaces and low-dimensional systems. Particular attention is paid to systems of nanometer size. Together with the theoretical activity, in which most of the research is focused, experimental work based on scanning tunnelling microscopy (STM) and photoemission techniques is developed in the nanophysics laboratory. In general, the group concentrates on the following areas of research:

- **Structural and electronic properties** of materials using first-principles methodologies. Among other systems, bulk materials, surfaces, metal clusters, molecules of biological interest, and nanowires, have been recent targets of study.
- **Electron dynamics** in solids, surfaces, adsorbates, and low-dimensional systems, with particular emphasis on ultrafast processes and size effects.
- **Theoretical and experimental analysis** of tunnelling topography and spectroscopy in nanostructures.
- **Interaction of charges and radiation** with surfaces and nanostructures: nanophotonics, theory of photoemission and ion-solid interactions, and electron microscopy.

Polymers and Non-crystalline Materials

The current activities in this area are focussed on the general line: Structure and Dynamics of polymer materials and glass-forming systems. This is mainly an experimental approach by combining different techniques, in particular, neutron scattering, broadband dielectric spectroscopy and nuclear magnetic resonance. Moreover, we are also developing atomistic molecular dynamics simulations of polymer systems and coarse-grained methods as well. Within this general area, we can identify the following recent topics of research:

- Dynamics of nanocomposites and multicomponent polymer materials.
- Development of simulation methods in polymers.
- Dynamics of glass-forming polymers and the problem of the Glass Transition.
- Molecular rheology of branched polymers.
- Water-polymer interactions: a new route to approach water behaviour in biological systems.
- Confinement effects in polymer blends and multicomponent systems.
- Relationship between transport properties and molecular mobility in polymeric membranes.

SCIENTIFIC HIGHLIGHTS

The following articles show a sampling of the main topics of research at DIPC.

2004/05

Deconfinement In a Two-dimensional Optical Lattice

by *A.F. Ho*[1], *M.A. Cazalilla*[2] *and T. Giamarchi*[3]

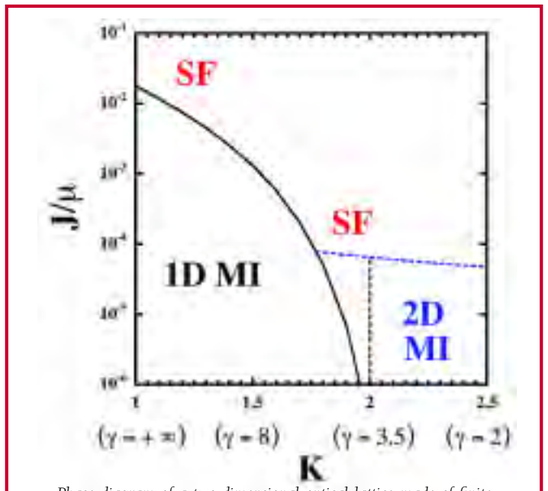
As it was experimentally demonstrated ten years ago, in three dimensional space, bosons can undergo Bose-Einstein condensation, that is, they can reside in the same quantum state. However, when confined in a one-dimensional structure, such a phenomenon becomes impossible. Furthermore, a periodic potential and boson-boson interactions can both conspire to localize the atoms in an insulating state known as Mott insulator. We investigate how the transition between these different states takes place in a system of bosonic atoms confined in an anisotropic optical lattice.

In 1924, Albert Einstein received a letter from an entirely unknown Indian physicist, S.N. Bose. By that time, Einstein had been already awarded a Nobel prize, and was well known and famous even to the general public. Enclosed with Bose's letter, there was a manuscript, for which Bose requested Einstein's assistance for its translation and submission to a renowned German journal, *Zeitschrift für Physik*. In his manuscript, Bose presented a statistical method that he applied to the study of radiation, demonstrating how to obtain Planck's radiation formulas from the basic assumption of the existence of light quanta ("photons") put forward by Einstein himself twenty years earlier. Einstein quickly realized the importance of the work of his Indian colleague, and not only did he prepare a translation and submitted it to the journal, but also found a nice extension to Bose's work. This is how he came across the phenomenon called Bose-Einstein condensation (BEC): Einstein noticed that, by applying Bose's statistical rules to atoms (instead of photons, as Bose had done), the atoms should undergo an interesting transition at sufficiently low temperatures. Indeed, whereas at high enough temperature a gas of atoms described by Bose statistics would entirely behave as a classical gas, as the temperature decreases, the behavior would become qualitatively different, and eventually, below a certain temperature, most of the atoms would reside in the same (quantum) state. Almost seventy years later, BEC was observed in a diluted gas of alkali atoms, cooled down to temperatures of about one millionth of degree above the absolute zero (–273.16 degrees Celsius). It happened just as Einstein had predicted using Bose's methods.

Nevertheless, it is interesting to note that Einstein's results apply only for an atomic gas in three spatial dimensions (3D). When one examines the conditions for Bose-Einstein condensation for a gas confined to move in a narrow tube, that is, in one dimension (1D), one reaches the surprising conclusion that BEC cannot occur. In fact, if atoms did not interact at all, BEC would only happen exactly at the absolute zero of temperature. However, with interactions things get worse, since they make the motion of all atoms in 1D correlated, pretty much like the motion of cars in a traffic jam is correlated. As a consequence, BEC in 1D cannot take place even at the absolute zero. However, in view of the above discussion, one question immediately arises: What happens when we go from 1D to 3D? First we have to think of a set up where such an experiment can be done. Miraculously, this has been rendered possible recently thanks to advances in laser manipulation of the same cold alkali gases where BEC was observed in 1995. During the last few years, several experimental groups in Europe and the US have been able to create light interference patterns (a sort of hologram) where one can tightly trap alkali gas atoms in tubes, thus confining their motion to 1D. The force that confines the atoms arises due to the AC Stark effect, i.e. the laser electric field induces a dipole on the atom, which in turn responds to the same electric field by moving to regions where the electric field is low (or large, depending on the laser frequency). The confinement thus attained can be made very tight, such that atoms cannot escape from the tubes but, by decreasing the intensity of the lasers that create the hologram, hopping of atoms from tube to tube can be allowed.

In our article, we mapped out the possible phases (i.e. states of matter) of such a system of weakly coupled tubes. The results uncover the astonishing behavior of strongly correlated quantum matter that can only be observed at temperatures very close to the absolute zero. The competition between the tendency of atoms to gain kinetic energy, and therefore become delocalized, and the tendency to become localized due to their mutual interaction is exhibited by the different phases where the system can be found. We find that not only can the system become a very exotic type of Bose-Einstein condensate (denoted SF in the figure), with very anisotropic properties, but it also exhibits two kinds of Mott insulating phases (1D MI and 2D MI), where the behavior of atoms is dominated by their mutual interactions. What is interesting about cold atomic gases in optical lattices is that the parameters of the system can be changed in a continuous and highly controllable way. Thus, almost at the same time that we carried out our calculations, Tilman Esslinger and his group at the legendary ETH in Zurich (the place from where Einstein himself got his BS and PhD degrees in Physics) were carrying careful experiments that demonstrated that the phases that we predicted are actually observed in the experimental systems. ■

REFERENCE
A.F. Ho, M.A. Cazalilla, and T. Giamarchi, *Physical Review Letters* **92**, 130405 (2004).



Phase diagram of a two-dimensional optical lattice made of finite one-dimensional gas tubes filled with bosonic atoms. The region labeled SF corresponds to parameter range where an anisotropic Bose-Einstein condensate is stable. The region labeled as 1D MI corresponds to the Mott insulating phase, where atoms are localized at the minima of a periodic potential. The 2D MI phase corresponds to a state where the atoms are localized within the gas tubes, but not by the periodic potential.

We find that not only can the system become a very exotic type of Bose-Einstein condensate, with very anisotropic properties, but it also exhibits two kinds of Mott insulating phases, where the behavior of atoms is dominated by their mutual interactions.

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Complete Photo-fragmentation of The Deuterium Molecule

by *Th. Weber[1,3,5], A. Czasch[1], O. Jagutzki[1], A. Müller[1], V. Mergel[1], A. Kheifets[2], E. Rotenberg[3], G. Meigs[3], M.H. Prior[3], S. Daveau[3], A.L. Landers[4], C.L. Cocke[5], T. Osipov[5], R. Díez Muiño[6], H. Schmidt-Böcking[1] and R. Dörner[1]*

All properties of molecules—from binding and excitation energies to their geometry—are determined by the highly correlated initial-state wavefunction of the electrons and nuclei. Details of these correlations can be revealed by studying the break-up of these systems into their constituents. The fragmentation might be initiated by the absorption of a single photon, by collision with a charged particle or by exposure to a strong laser pulse: if the interaction causing the excitation is sufficiently understood, the fragmentation process can then be used as a tool to investigate the bound initial state. The interaction and resulting fragment motions therefore pose formidable challenges to quantum theory.

A 'complete' description of the break-up of a molecule

In the article by Weber *et al.*, the coincident measurement of the momenta of both nuclei and both electrons from the single-photon-induced fragmentation of the deuterium molecule is reported. For each charged particle, the position of impact on the detector and the overall 'time of flight' are measured, and from them the initial momentum of all four particles can be deduced directly. Even more excitingly, in the case of hydrogen, the ions leave in opposite directions so quickly (compared with their rotational motion) that even the alignment of the molecular axis can be determined with respect to the polarization direction of the incident light. From the kinetic energy of the nuclei arriving at the detector, one can also obtain the Coulomb potential associated with their initial separation. Quantum mechanically, one maps the nuclear vibrational wave function onto the Coulomb potential to yield a kinetic-energy spectrum. All this gives a three-dimensional 'photograph' of the Coulomb explosion.

The results reveal that the correlated motion of the electrons is strongly dependent on the inter-nuclear separation in the molecular ground state at the instant of photon absorption. Although multiple scattering of the photoelectron wave could lead to a variation of the angular distributions, calculations for this particular system show that this effect, as a function of the inter-nuclear separation, is rather small. This is because the protons are relatively weak scattering centres and the long wavelength of the photoelectrons would require long paths within the molecular potential. The ultimate reason for such strong dependence should be then found in the initial-state wave function features. The experimental results are thus highly sensitive tests of the initial-state wave function and, consequently, of electron correlation effects in the initial state. ■

REFERENCE

T. Weber, A.O. Czasch, O. Jagutzki, A. K. Müller, V. Mergel, A. Kheifets, E. Rotenberg, G. Meigs, M.H. Prior, S. Daveau, A. Landers, C.L. Cocke, T. Osipov, R. Díez Muiño, H. Schmidt-Böcking, and R. Dörner, *Nature* **431**, 437 (2004).

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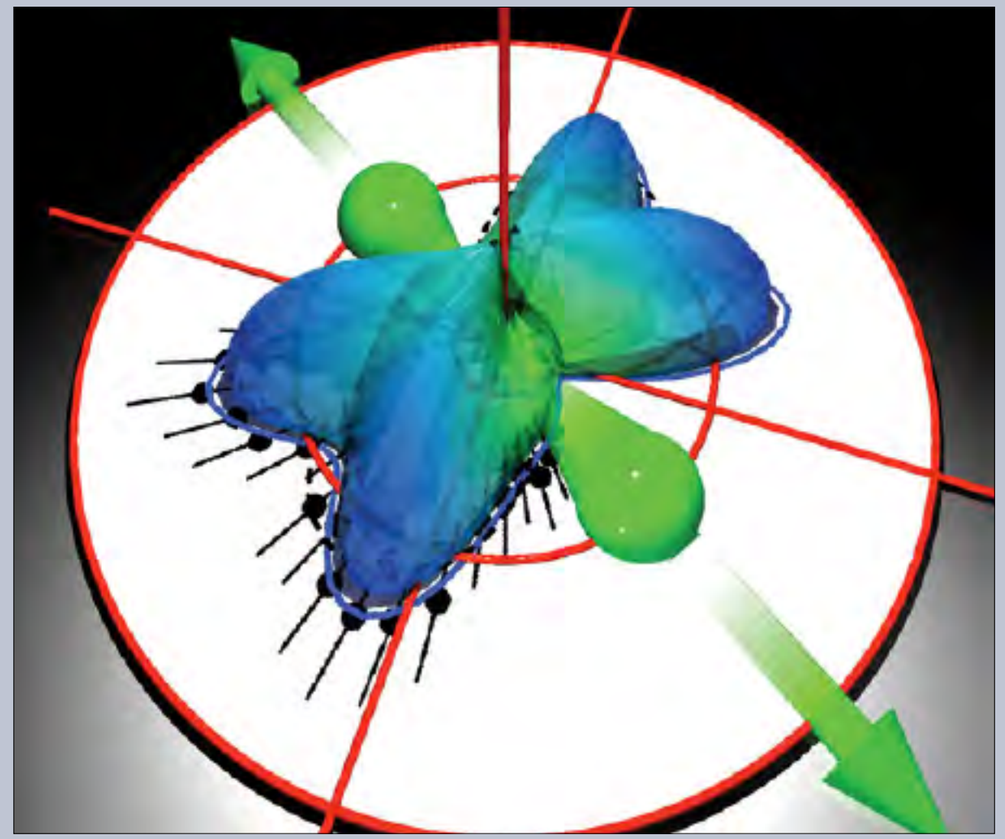

A three-dimensional 'photograph' of the double ionization of deuterium molecules, initiated by the absorption of photons.

The results reveal that the correlated motion of the electrons is strongly dependent on the inter-nuclear separation in the molecular ground state at the instant of photon absorption.

Contrast Reversal And Shape Changes of Atomic Adsorbates Measured with Scanning Tunneling Microscopy

by *F. Calleja[1], A. Arnau[2], J.J. Hinarejos[1], A.L. Vázquez de Parga[1], W.A. Hofer[3], P.M. Echenique[2,4] and R. Miranda[1]*

Systematic, quantitative comparisons between STM experiments and first principles simulations of O(2 x 2)/Ru(0001) have been performed. The shape of the atomic adsorbates in the images depends strongly on the tunnelling resistance and changes reversibly from circular (high resistance)to triangular (low resistance). In addition, after adsorption of oxygen on the STM tip we observe a contrast reversal on the surface, confirmed by extensive numerical simulations.

In many exciting areas, e.g. catalysis, high Tc materials and other complex transition metal oxides, it is important to identify metal and oxygen sites at surfaces in order to understand processes such as dissociation of molecules, spatial inhomogeneities in the superconducting gap or the role of impurities in the formation of striped phases. Although Scanning Tunnelling Microscopy (STM) images can in principle be used to characterize the topography of surfaces at the atomic level, they do not always simply reflect the real position of surface atoms. If we restrict ourselves to adsorbed oxygen layers or oxide surfaces, there are experimental reports claiming that, depending on the system and the state of the tip, either the O or the metal atoms are the bright features in the STM images. The observed shape of images is well understood in the case of isolated oxygen atoms adsorbed on metal surfaces. However, in dense, ordered arrays of adsorbed oxygen the situation is still unclear. Because the geometric and electronic structure of the surface, as well as the chemical state of the tip, play a role in determining the corrugation, contrast and shape of the image, it is necessary to perform *ab-initio* calculations to interpret properly the STM images. Here we report on a fundamentally new level of comparison between experiment and theory to clarify the role of the different parameters determining STM images like tip structure, sample voltage (V), tunneling current (I), and gap resistance (R). The measured series of STM images of the model system, O(2x2) superstructure of Oadsorbed on Ru(0001), is shown to be in quantitative agreement with first principles simulations. The geometric structure (adsorption site, interatomic distance, and relaxations) of the chosen system has been carefully characterized by low energy electron diffraction (LEED). The control parameters of the operation of the STM were systematically varied over a broad range (10 mV<V <1 V, 0:03 < t < 50 nA, 300 kOhm<R < 2 GOhm), and the ensuing changes were recorded and compared to simulated images. ■

REFERENCE

F. Calleja, A. Arnau, J.J. Hinarejos, A.L. Vázquez de Parga, W.A. Hofer, P.M. Echenique and R. Miranda, *Physical Review Letters* **92**, 206101 (2004).

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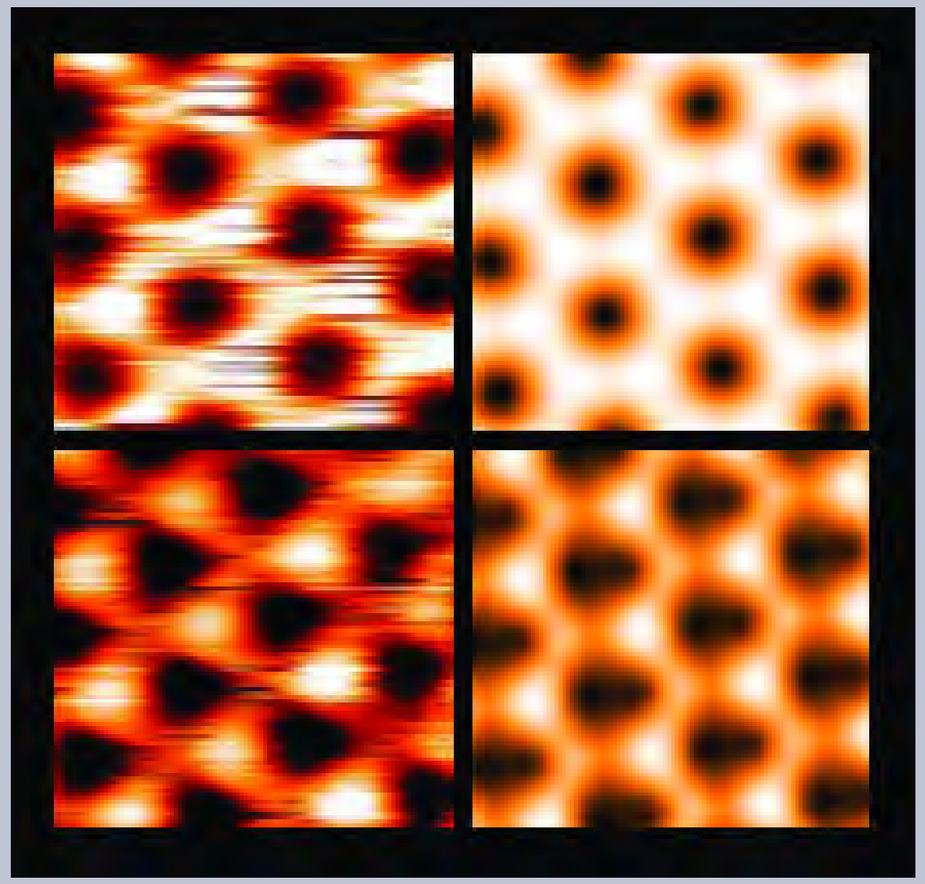
3 Surface Science Research Centre, University of Liverpool, UK
4 Donostia International Physics Center, San Sebastian, Spain



Comparison of experimental (left) and simulated (right) STM images of O(2x2)/Ru(0001). In both cases the sample voltage was -30 mV. The simulations have been performed with tunnelling currents of 0.03 nA (above) and 0.3 nA (below) and agree with the experiments.

Band Structure versus Dynamical Exchange-correlation Effects in Surface Plasmon Energy and Damping:

A First-Principles Calculation

by *V.M. Silkin*[1], *E.V. Chulkov*[1,2], *and P.M. Echenique*[1,2]

Since the introduction of surface plasmon (SP) concept remarkable progress has been achieved in the understanding of collective electronic excitations at metal surfaces. These excitations play an important role in such areas as surface dynamics including one-particle (electron and hole) dynamics, SP microscopy, SP resonance technology as well as in photonic applications. Here we report on the results of a first-principles parameter-free calculation of the dynamical surface response and surface plasmon properties of magnesium, a prototype simple metal. We demonstrate that band structure effects have a more profound impact on the SP properties than dynamical exchange correlation. Nevertheless to obtain better agreement with experiment the inclusion of proper exchange-correlation kernel is needed.

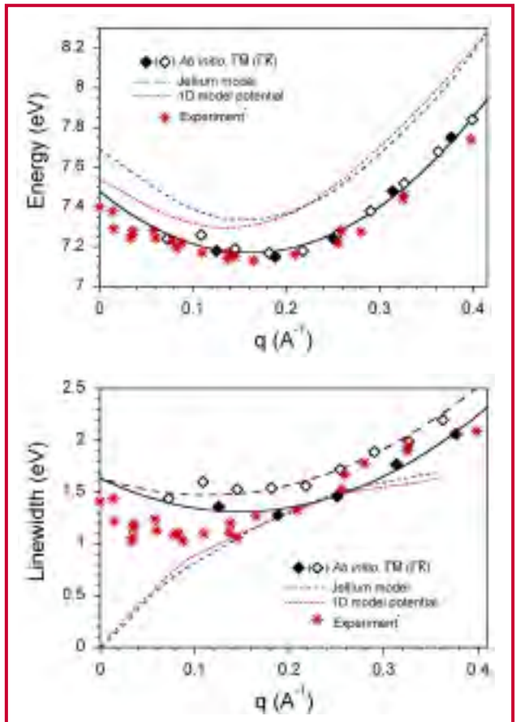
Surface plasmon properties are important in many areas of surface science.

Conceptually the SP, a fundamental surface mode, can be traced to the peaks of the imaginary part of the surface response function derived from the density response function of the interacting electron system. The density response includes both bulk and surface electrons and represents a very complex interplay between one particle electron states (band structure) and dynamical many-body correlations that affects both the SP energy and linewidth.

The difficulty in the description of a SP stems from a gradual transition of main driving forces from the long-wavelength limit to large momenta. In the long-wavelength limit the dielectric response is controlled by bulk properties, while for large momenta the main effect is due to the surface dielectric response. Thus for the proper description of the dispersion of the SP energy and width it is necessary to include both the bulk and surface electronic structure on the same footing. In parallel with the band structure the exchange-correlation effects were shown to be important for the description of bulk collective excitations in simple metals. For surface collective excitations the incorporation of dynamical exchange-correlations might be even more important than for bulk materials since unlike the bulk the surface charge density experiences fast variation at short distances from bulk values to zero in vacuum.

In the article by Silkin *et al.*, the results of the first parameter free ab initio calculation of the SP energy and linewidth for a real metal surface are reported. The relative impact of band structure and dynamical exchange-correlations on the SP is studied for Mg(0001). This surface can be viewed as a test one for the comparison of theoretical and experimental results because of the best quality of the Mg single crystal surface with respect to other simple metals. The results obtained show that even for such a nearly-free electron metal as Mg an excellent agreement with the experimental SP energy and linewith in a large range of 2D momenta is found if both the bulk and surface band structure on the same footing together with dynamical exchange-correlations are taken into account. The inclusion of band structure into the theory is crucial for the description of the correct behavior of the SP linewidth as well as of its anisotropy.

The calculated SP dispersion and linewidth for two symmetry directions of surface Brillouin zone are shown in the figure together with the experimental data. We also show there the results obtained from the jellium and one-dimensional potential models. From the comparison of these three models one can discriminate the relative role of such factors as modulation of one-electron potential in the direction perpendicular to the surface and full inclusion of three-dimensional band structure effects. In particular, the latter are crucial for the description of the SP linewidth, whereas jellium and one-dimensional potential models fail to reproduce the experimental linewidth for both small and large momenta. These effects account for the significant anisotropy predicted for the SP linewidth. They are also important for the energy dispersion of the SP. The inclusion of the momentum dependent exchange-correlations improves the theoretical results leading to excellent agreement with the experimental data. We have also found that lateral crystal local field effects have a negligible impact on the SP properties. Our conclusions about the relevance of band structure can be extended to systems with more complicated electronic structure than magnesium, for instance, to silver surfaces, which are of particular interest due to an unusual energy and dispersion of surface plasmon, and to palladium surfaces. ■



Surface plasmon energy (above) and linewidth (below) dispersions for Mg(0001) calculated with momentum-dependent kernel. Ab initio data for $\bar{\Gamma}\bar{M}$ ($\bar{\Gamma}\bar{K}$) direction of surface Brillouin zone are shown by the filled (open) diamonds. Solid (long dashed) line is the corresponding best fit to the data. Dashed (dotted) lines present the jellium model (1D model potential) diversions.

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On the base of ab initio calculations it was demonstrated the relative importance of electron band structure and dynamical exchange-correlations in surface plasmon energy and its linewidth.

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Lifetimes of Excited Electrons in Fe and Ni: First-principle GW + T-matrix Theory

by *V.P. Zhukov*[1], *E.V. Chulkov*[1,2] *and P.M. Echenique*[1,2]

We develop a first-principle method for evaluating the life-times of spin-polarized excited electrons in ferromagnetic metals. The calculations show that the decay of low-energy excited states is expressly spin-dependent, in particular in Fe, where the life-time of spin-minority states is reduced due to the emission of magnons and spin-flip electron-hole pairs.

The spin-asymmetry of the excited electron life-times is a phenomenon that makes possible triggering of current in spintronic devices.

The spin-dependent lifetime of excited electrons in ferro-magnetic materials characterizes the ability of electrons to transfer the spin and is important for transport and spin accumulation phenomena employed in novel spintronic devices. It has been studied experimentally, by means of photoemission and time-resolved two-photon photoemission spectroscopy, and theoretically, mainly within semi-empirical models of scattering theory. However, present methods of evaluating the electronic lifetimes in ferromagnetic materials are still far from being perfect. In particular, an essential drawback of the semi-empirical theoretical calculations is the invocation of adjustable parameters and omission of some important mechanisms of the fast electron decay, such as the generation of electron-hole Stoner's pairs and spin waves.

A good alternative to the methods having the origin in scattering theory is provided by the *ab initio* methods based on many-body theory. The most important of them is the GW approach, where the lifetime is evaluated from the imaginary part of the electron self-energy. This approach is fairly good for systems with long-range screening, but it fails to describe short-range interactions and neglects the spin-flip scattering processes. In order to achieve a better understanding of the fast electron decay in ferro-magnetics, we extended the GW method by including the multiple scattering processes evaluated within the T-matrix approach.

We define T-matrix operator as a solution of Bethe-Salpeter equation

$$T_{\sigma_1\sigma_2}\langle 1,2|3,4\rangle = W(1,2)\delta(1-3)\delta(2-4) + W(1,2)\int d1'\,d2'\,K_{\sigma_1\sigma_2}\langle 1,2|1',2'\rangle T_{\sigma_1\sigma_2}\langle 1',2'|3,4\rangle$$

with the static RPA screened potential W. The kernel of this equation K is a product of two spin-dependent Green functions

$$K_{\sigma_1\sigma_2}\langle 1,2|1',2'\rangle = G_{\sigma_1}(1,1')G_{\sigma_2}(2',2)$$

In our calculations all the possible combinations of G have been taken into account: electron-electron, electron-hole and hole-hole Green's functions with equal and different spins. The most important T-matrix contribution to the self-energy is the direct term

$$\Sigma_{\sigma_2}(4,2) = -\sum_{\sigma_1}\int d1d3 G_{\sigma_1}(3,1)T_{\sigma_1\sigma_2}\langle 1,2|3,4\rangle$$

With $\sigma_1=\sigma_2$ we have high-order contributions to the non-spin-flip scattering, with $\sigma_1-\sigma_2$ this term provides spin-flip Stoner and spin-wave contribution to the self-energy. The pole frequencies of T-matrix with $\sigma_1-\sigma_2$ correspond to magnon energies. The explicit equations for the self-energy Σ^d in moment and frequency representation have been derived and implemented based on LMTO band-structure method.

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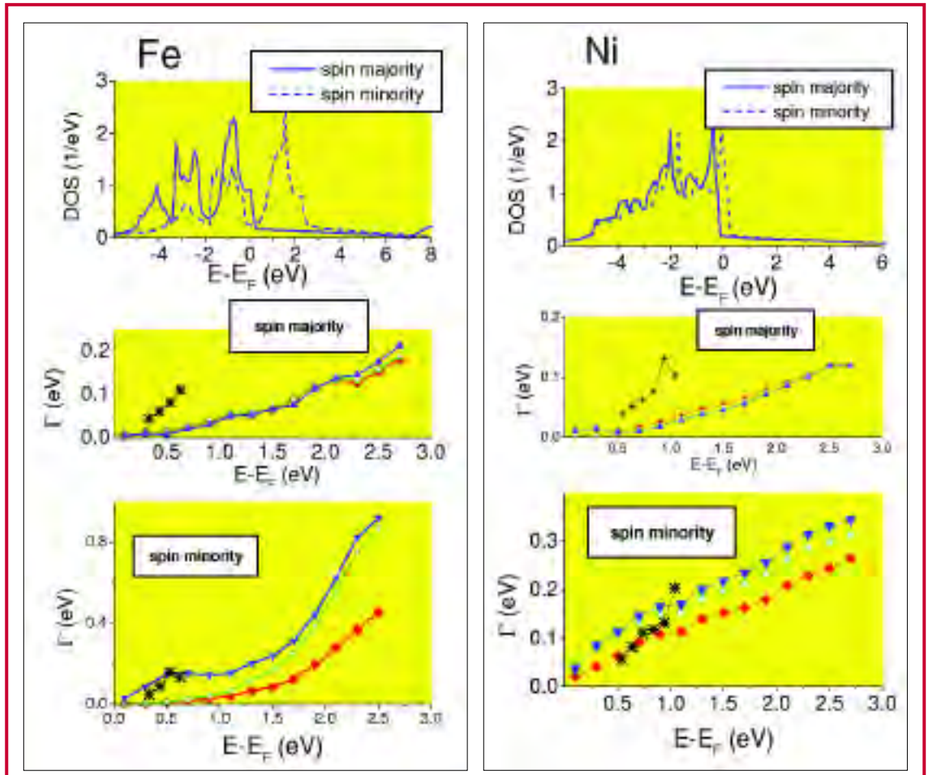

Figure: The calculated and experimental inverse lifetimes Γ of excited electrons in Fe and Ni. Solid red diamonds show the GW contribution to Γ, open green circles show GW+T non-spin-flip contribution, and red triangles show complete GW+T(non-spin-flip + spin-flip) Γ-values. Black stars show the experimental TR-2PPE inverse lifetimes.

In the Figure we show the calculated spin-projected densities of states (DOS) and inverse lifetimes (Γ) for Fe and Ni. For the spin-majority excited electrons both in Fe and Ni the contribution of T-matrix terms to Γ appear to be small. But for spin-minority electrons the effects of both spin-flip and non-spin-flip T-matrix terms are essential. For spin-minority electrons in Fe at excitation energy about 0.5 eV we observe a strong deviation of the GW+T results from the GW results. This deviation is associated with the scattering of excited electrons accompanied by the generation of spin waves and Stoner's electron-hole pairs. Similarly, the GW+T results for spin-minority electrons in Ni at excitation energy below 0.5 eV also diverge from GW results, but this divergence is associated mainly with the multiple electron-hole scattering without spin flips. The Γ values calculated for spin-minority electrons are in good agreement with experimental TR-2PPE data. But the theoretical Γ values for spin-majority states in Fe and Ni still remain lower than the experimental data. This is consistent with the fact that the experimental data include the effects of transport, electron-impurity and electron-phonon scattering. ■

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Strong Spin-orbit Splitting on Bi Surfaces

by *Yu. M. Koroteev[1,2], G. Bihlmayer[3], J.E. Gayone[4,5], E.V. Chulkov[1,6], S. Blügel[3], P.M. Echenique[1,6], and Ph. Hofmann[4]*

Understanding of electronic properties of surfaces of heavy semimetal materials is of paramount importance for transport phenomena due to the spin-orbit splitting of surface states (SS). Here we present the first ab initio calculation together with angle-resolved photoemission measurements of the SS bands on low-index surfaces of Bi. We show that the spin-orbit interaction leads to a strong splitting of the SS bands and profound modifications of the dispersion of these states and the corresponding Fermi surfaces. The implications of these findings can be important for the surface screening, surface spin-density waves, electron (hole) dynamics in surface states, quasiparticle interference, and for possible applications to the spintronics.

Surface states (SS) of a semimetal would give a prominent contribution to surface density of states that could make these systems interesting for applications in spintronics. The surfaces of the semimetal Bi are ideal to advance our understanding of spin-orbit coupling (SOC) on surfaces and how it manifests in experiments on electron-phonon coupling, electron and hole dynamics, possible formation of surface charge and spin density waves, and in quasiparticle interference. The strong SOC in low-dimensional structures of non-magnetic materials could also have applications like spin-filter devices.

We show by combining the results of first-principles calculations with high-resolution measurements of the electronic structure by ARPES that the SS on low-index surfaces of Bi exhibit a spin-orbit splitting of the bands which is by far stronger than any case reported so far. The results of the calculation agree well with experiment but only if the SOC is taken into account. We find that the SOC induced splitting is an essential ingredient for the description of the electronic structure: it profoundly changes the SS dispersion and the corresponding Fermi surfaces on all the Bi surfaces of interest.

Figure 1 shows the electronic structure of Bi(111) together with the projected bulk band structure calculated with and without

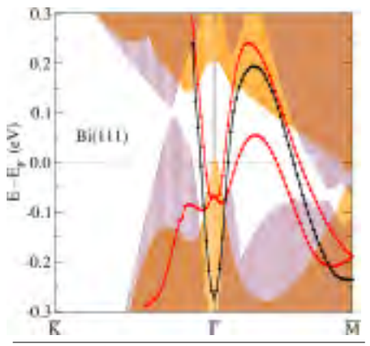

Figure 1. Surface states of Bi(111) calculated without (black) and with (red) spin-orbit splitting included. The shaded areas show the projection of the bulk bands obtained without (violet) and with (yellow) SOC and their superposition (brown).

SOC. Without SOC, we find a parabolic $\bar{\Gamma}$ SS located in the nonrelativistic energy gap. Around $\bar{\Gamma}$ this SS band gives an electron FS hexagon. With the SOC included it results in a spin-splitting of the SS in all the symmetry directions and leaves it degenerate only at $\bar{\Gamma}$ and at $\bar{M}$. Around $\bar{\Gamma}$ this relativistic SS is degenerate with bulk states and shows less clear surface character. The lift of the spin degeneracy leads to radical change of the surface FS: 1) The radius of the FS hexagon is

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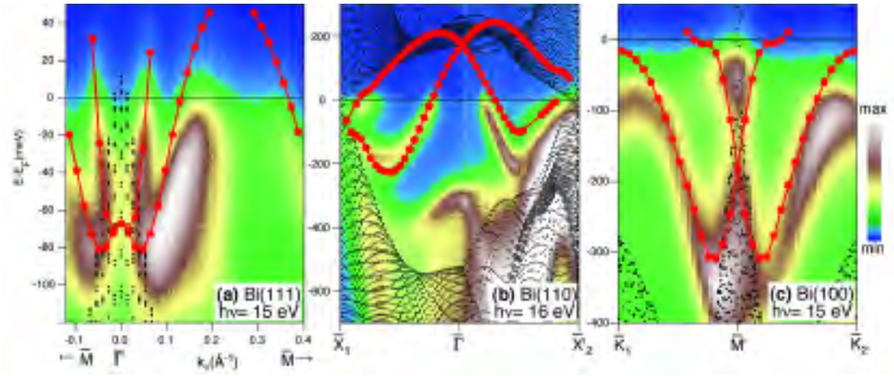

Figure 2. Calculated and measured electronic structure in the vicinity of two high symmetry points on three surfaces of Bi. (a) $\bar{\Gamma}$ on Bi(111), (b) $\bar{\Gamma}$ on Bi(110), and (c) $\bar{M}^1$ on Bi(100). The small black dots are the projected bulk band structure. The red filled circles are the calculated surface state energies, thin red line is a guide to the eye. The photoemission intensity is linearly scaled from dark blue (minimum) to white (maximum).

smaller by 30% compared to the nonrelativistic calculation; 2) In the $\bar{\Gamma}$ $\bar{M}$ symmetry directions the hole lobes are formed. Another remarkable feature of Bi(111) is the very strong anisotropy of the SOC: it is 0.2 eV in the $\bar{\Gamma}$ $\bar{M}$ direction and even more in the $\bar{\Gamma}$ $\bar{K}$ one.

The strong spin-orbit splitting is verified by comparing the calculations with the experimental results. Figure 2 shows the calculated electronic structure for Bi surfaces together with experimental data. In Figure 2(a) we find excellent agreement for the two split SS for Bi(111). Figure 2(b) also shows the situation for Bi(110). In contrast to Bi(111) this SS is unoccupied at and has negative effective electron masses that lead to the formation of the hole FS pocket around $\bar{\Gamma}$. The scenario of a very steep band and a flatter one near $\bar{\Gamma}$ can be found on Bi(100).

The SOC-induced splitting should have some important consequences for the physical properties of the Bi surfaces, in particular, for the screening. In the Lindhard picture of screening, the susceptibility (q) is given by an integral over all processes where an electron hops between an occupied state and an unoccupied state separated by q. In a two-dimensional situation this type of screening can lead to a CDW-type instability only when there are 'nested' elements of the FS, separated by q. Such a situation exists for Bi(111) where the FS of the electron pocket around $\bar{\Gamma}$ is hexagonal. Ast and Hoöchst have recently shown (*Physical Review Letters* **90**, 016403 (2003)) that the leading edge of the energy distribution curves at the Fermi level crossing shifts discontinuously as a function of temperature, indicating the formation of a CDW. However, when we take into account the spin of the states involved in the alleged formation of the CDW, the electron hopping across the FS would have to undergo a spin-flip because of the split nature of the bands. This makes the occurrence of a CDW very unlikely.

The spin-orbit splitting in surface bands on the Bi surfaces can also have drastic consequences for electron and hole dynamics in surface states. In particular, the surface response function should include all the spin-flip processes between the split surface bands with different spin direction. It can lead to the formation of surface spin-density waves even in cases when the nesting at the surface FS does not occur. The spin-orbit splitting should also lead to different hole (electron) lifetimes in surface states compared to that for the non-split surface state. This is due to both the surface response function that now includes spin-flip processes and to a different phase space factor. The surface state spin-orbit splitting can also affect the electron-phonon (e-ph) coupling on the Bi surfaces. We would like to note that the existence of spin split surface states also permits a spin-wave mediated e-ph interaction. ■

The surface response function should include all the spin-flip processes between the split surface bands with different spin direction.

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Controlling the Conductance of Single-walled Carbon Nanotubes: Anderson Localization

by *C. Gómez-Navarro[1], P. J. de Pablo[1], J. Gómez-Herrero[1], B. Biel[2], F. J. García-Vidal[2], A. Rubio[3], and F. Flores[2]*

Carbon nanotubes are a good realization of one dimensional crystals where basic science and potential nanodevice applications merge. For the case of electronic circuits based on carbon nanotubes, the influence of disorder and defects is of fundamental relevance in the performance of the device (e.g. the density of defects can change the transport regime from ballistic regime to either weak or strong localization). Defects can be present in as-grown carbon nanotubes therefore, it is crucial to understand the properties of these defects in order to conquer their detrimental effects, but also because controlled defect introduction may be used to tune nanotube properties in a desired direction.

Observation of Anderson localisation at room temperature in irradiated carbon nanotubes

Quantum theory dictates that for a one dimensional conductor with defects weak localization effects emerge when the "phase coherence length" is larger than the localization length, L_0. For very long wires ($L>>>L_0$), the electron transport is a diffusive process controlled by localization, with the electrons hopping between neighbouring localized states. However, if L is not too large (for L about 3-10 L_0) and the inelastic interaction is weak, the wire resistance is controlled by the phase-coherent electron propagation, falling into the strong localization regime in which the resistance increases exponentially with the length of the wire. This regime is the one addressed here as in nanotubes the dephasing length can easily be longer than the localization length, which is the basic requirement for achieving Anderson localization.

Experimentally, a metallic AFM tip was used to measure the current vs. voltage characteristics of the nanotubes as a function of the distance between the metallic AFM tip, used as mobile electrode, and a fixed macroscopic gold electrode (see figure). By measuring the electrical resistance of the same metallic nanotube after successive irradiations we were able to map the resistance as a function of the nanotube length. Our data shows that the resistance increases exponentially with length at scales L ≥ 500 nm (see inset in the figure). The length scale at which this exponential behavior is observed could be reduced substantially by irradiation with Ar^+ ions, indicating that it is caused by Anderson localization. Simulations demonstrated that mainly di-vacancies contributed to the exponential conductance drop induced by irradiation (di-vacancies appear in about 30-40% of the Ar^+ impacts).

We used a first-principles Local Orbital Density Functional method to calculate the relaxation around the defects and transport characteristics. The advantage of this approach is that it provides a means of calculating the conductance using standard Green-function techniques derived for tight-binding Hamiltonians but now with first-principles accuracy allowing the calculation of the electronic properties of very long nanotubes (up to several microns long) with an arbitrary distribution of defects immersed on them providing a quantitative comparison between theory and experiments. In the figure we show the calculated mean value of the room T resistance (as a result of an average over 15 random cases) as a function of the carbon nanotube length for different d's.

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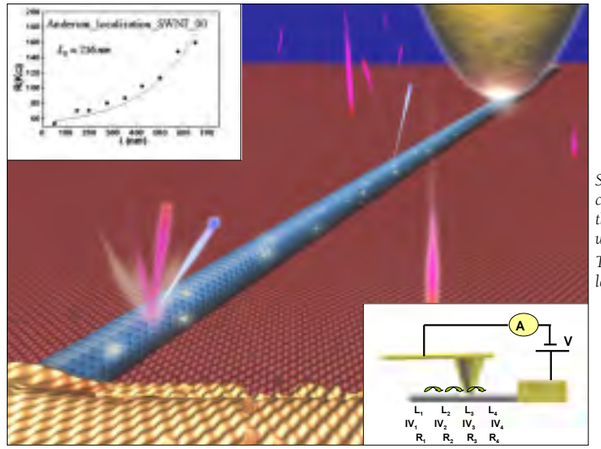

Scheme of the experimental set-up showing a gold covered AFM tip, the macroscopic gold electrode, the SWNT, the irradiation with Ar atoms and the used circuit.
The top inset shows one low-voltage-resistance vs. length, clearly exhibiting Anderson localisation.

The calculated resistance fits a universal curve once it is plotted in terms of the number of defects (N) instead of the total length (L). The inset shows that calculated room T localization length, L_0 exhibit two distinct regimes: i) for lower defect density (i.e., large values of *d, d*>5 nm), L_0 depends linearly with *d*, ii) For higher defect density (small values of *d*), L_0 saturates. In all our measurements the defect density is below 0.15% corresponding to case (i).

To highlight our findings, we have shown the extreme importance of defects (in particular di-vacancies) on the low-bias conducting properties of single-walled carbon nanotubes irradiated with an Ar^+ ion beam: only a 0.03% of di-vacancies produce an increment of three orders of magnitude in the resistance of a 400 nm carbon nanotube segment. Our theoretical calculations support this conclusion, indeed for a (10,10) carbon nanotube we have found: (i) the transition between the ballistic and the localization regimes appears for a small number of di-vacancies (about 3–5). (ii) For a higher number of defects the system shows localization, reducing the number of effective channels from two (ballistic) to one. (iii) At zero T, the nanotube conductance shows strong fluctuations. The net effect of a finite T is to wash out those strong fluctuations. We remark that, in spite of the disappearance of the fluctuations, the exponential behavior is still preserved at room T. Besides its fundamental relevance, this work opens new paths to tailor the electrical properties of future nanotube devices using ion irradiation. It also suggests the possibility of using these devices as radiation detectors and points out the limits of performance of carbon nanotubes in the presence of radiation. Whether interaction effects — that is, Tomanaga–Luttinger-liquid type of correlations — play a role has to be resolved by future investigation. ■

Temperature washed out the quantum fluctioatins in the conductance but not the localisation phenomena.

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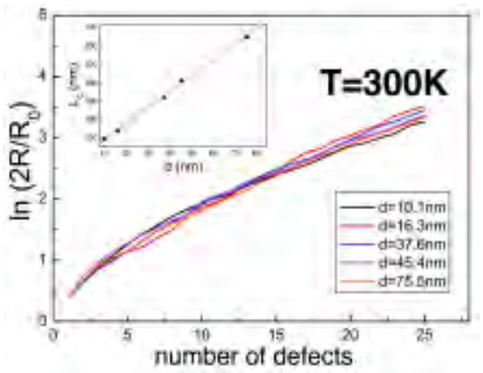

Interplay Between Electronic States and Surface Structure in Ag Layers

by *F. Schiller[1], J. Cordón[1], D. Vyalikh[2], A. Rubio[3,4,5], F.J. García de Abajo[5] and J. E. Ortega[3,4,5]*

We investigate the interplay between surface electronic states and geometric structure in the Ag/Cu triangular dislocation network. Experiments involve Scanning Tunneling Microscopy and Angle Resolved Photoemission with synchrotron radiation, and these are compared with model theoretical calculations. Distinct one-monolayer (incommnesurate) and two-monolayer (commensurate) lattices suggest the presence of structural instabilities that give rise to two-dimensional Fermi surface nesting and gap opening. Simple elastic/electronic energy arguments explain the experimental observations.

The interplay between electronic surface states and structure is observed in a Ag monolayer

Nanostructures exhibit exotic electronic and magnetic properties due to their reduced dimensions. New phases appear that do not have a bulk counterpart, e.g., *incommensurate* phases, which can drive structural phase transitions. They are particularly important in the context of cooperative phenomena like superconductivity, or spin and charge density wave transitions. Incommensurate phases appear upon Fermi surface nesting, i.e. by slightly forcing the crystal lattice to make the Fermi surface fit the Brillouin zone. This allows a band gap to open up at the Fermi energy, thereby lowering the electronic energy. The group at the Nanophysics Laboratory have recently provided clear evidence for Fermi surface nesting and surface state driven stabilization of the 2D incommensurate 9.5x9.5 Ag monolayer (ML) grown on Cu(111)[1].

The 1 ML Ag/Cu(111) system is an interesting example of layer-by-layer growth in large (13%) mismatched materials. In this case, the Ag monolayer wets the substrate and forms a compressed, out-of-registry 9.5x9.5 superstructure, with a lattice compression of 1.1% with respect to the bulk Ag(111) plane. The question arises why the system favors the out-of-registry 9.5x9.5 structure in this case, instead of, for instance, the registry 9x9 with only 0.4% lattice compression, which is indeed observed in 2 ML Ag/Cu(111). Using high resolution, angle resolved photoemission Schiller et al. have observed a Fermi gap to open in the out-of-registry 9.5x9.5 ML, by contrast to a gapless surface band observed in the registry 9x9 superstructure of the 2 ML Ag film. This result suggests that the compresed 9.5x9.5 incomensurate phase may be stabilized by such Fermi surface gap, and hence by the subsequent electronic energy gain.

Figure 1(a) shows the Scanning Tunneling Microcopy (STM) image for a ML thick Ag stripe grown on Cu(111) at 300 K. The work was carried out in the VT Omicron set-up in San Sebastian. The Ag is deposited on top of a Cu(111) single crystal held at 150 K and then shortly annealed to 300 K. This procedure leads to a hexagonal (see the Fourier

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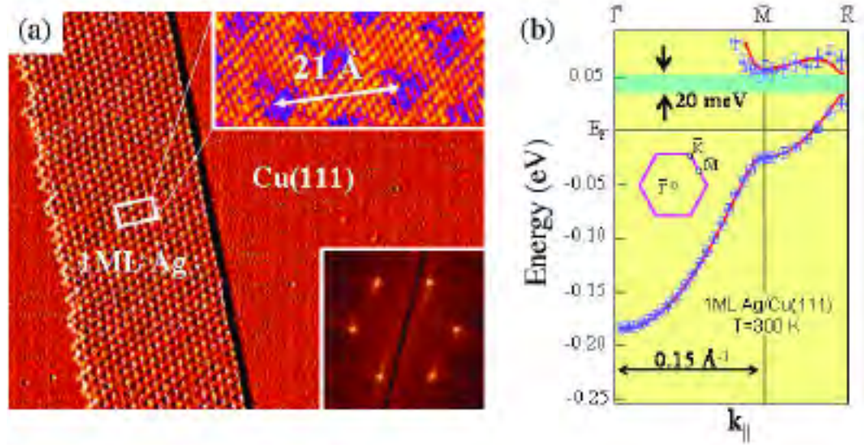

(a) STM image showing a monolayer-thick, Ag stripe grown on Cu(111). A 9.5x9.5 hexagonal pattern of lattice constant d=21Å is visible (Fourier transform in the lower inset). The upper inset shows a closer, atomically-resolved view. The structure is actually defined by a Ag close-packed layer that wets an array of triangular dislocation loops in the Cu(111) substrate.
(b) Surface bands for 1 ML Ag /Cu(111) measured with angle resolved photoemission (photon energy 21.2 eV). Fermi surface nesting leads to the large 80 meV Fermi gap that opens up at the bar point of the hexagonal structure. The surface band displays an absolute 20 meV slightly above the Fermi energy.

The group at the Nanophysics Laboratory have recently provided clear evidence for Fermi surface nesting and surface state driven stabilization of the 2D incommensurate 9.5x9.5 Ag monolayer (ML) grown on Cu(111).

transform in the lower inset) pattern with an average 21 Å lattice constant, i.e., a 9.5x9.5 reconstruction with respect to the Cu substrate. The atomically resolved image in the top inset probes the microscopic structure, namely a Ag close-packed layer that wets the array of triangular misfit dislocation loops induced in the Cu substrate. Figure 1(b) shows the surface band dispersion for 1 ML Ag/Cu(111) measured with angle resolved photoemission along the symmetry directions of the hexagonal structure. The photoemission experiments were performed with a Scienta 200 high-resolution angle resolved hemispherical analyzer in the University of Dresden. Fermi surface nesting at leads to the 80 meV band gap that opens up at that point.

The band dispersion measured across the whole Brillouin zone in Figure 1(b) shows strong modifications of the, otherwise, free-electron-like band of noble metals. In particular we observe a full 20 meV band gap slightly above the Fermi energy. The presence of this gap, which suggests exotic transport properties in the system, has been confirmed in a model calculation using a hexagonal array of triangular potential barriers[3]. On the other hand, using the band structure measured in Figure 1(b), the electronic energy difference between out-of-registry (9.5x9.5) and the registry (9x9) structures can be straightforwardly calculated. This gives a negative 0.31 meV/atom value, which indeed competes with the positive 0.48 meV/atom elastic energy difference, i.e., the energy needed to compress the Ag monolayer from the (9x9) to the (9.5x9.5) close-packed structures[2]. ■

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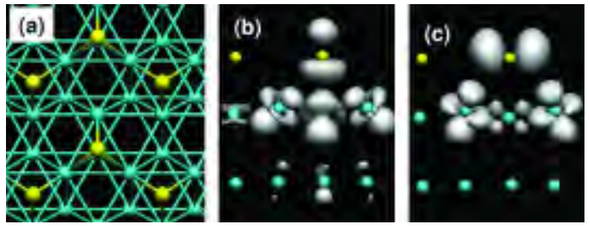
Direct Observation of the Electron Dynamics in the Attosecond Domain

by *A. Föhlisch*[1], *P. Feulner*[2], *F. Hennies*[1], *A. Fink*[2], *D. Menzel*[2], *D, Sánchez-Portal*[3], *P.M. Echenique*[3] *and W. Wurth*[1]

Two theoreticians from DIPC, Dr. Daniel Sánchez-Portal and Prof. Pedro M. Echenique, have recently participated in a study of the dynamics of electrons at surfaces that was published in *Nature*[1]. The aim of the study was to answer the following question:

How long does it take for an electron to hop between atoms?



For the studied system, an order structure of sulphur atoms deposited on the Ru(00001) surface, it turned out to be a very short time of about 320 attoseconds or 320x10^{-18} seconds. This is one of the shortest processes ever measured in solid state physics. However, the measurement was performed directly in time domain. This was only possible due to the use of an appropriate "clock", which in this case was chosen as the decay time of an internal hole of the sulphur atom. This technique is known as "core-hole-clock" spectroscopy, and in this work its resolution was significantly increased by the use of Coster-Kronig transitions. The experimentalist used X-ray pulses to excite an electron of sulphur to an electronic state where it is unstable and tends to move away from the sulphur atom into the ruthenium substrate. In this excited state the sulphur atom is also unstable against a Coster-Kronig autoionization process. This decay process takes place in a similar (although somewhat longer) time scale than the sulphur-ruthenium hopping, and produces a distinct signal that can be clearly measured. In fact, the autoionization produces two different signals (peaks) depending on whether the initial electron has already left the atom or not when the autoionization takes place. The key is then to measure the relative intensities of these two peaks, and the sulphur-ruthenium hopping time can be extracted from this intensity ratio. This measurement has been performed by a group of researchers from several German laboratories, the work being directed by Prof. Wilfried Wurth from Hamburg University.

The researchers from the DIPC simultaneously developed a method to calculate the charge-transfer times of electrons initially residing in excited states of adsorbates to the corresponding metallic substrates. The calculations were based on state-of-the-art electronic structure calculations, using the so-called density-functional theory, to compute the details of the combined adsorbate-substrate system. These results were then combined with calculations of the bulk of the substrate material to obtain the Green's function of the semi-infinite system using recursive techniques. The calculations are thus based on a realistic description of the electronic structure of both systems, the substrate and the adsorbate, and the interaction between them. This allows to make predictions about the charge-transfer rates in different systems and to understand in detail the dynamics of electrons at surfaces. This scheme was then applied to study the sulphur covered ruthenium substrate. It was confirmed that for the particular set-up used in the experiments, the charge-transfer time was indeed well below 1 femtosecond (10^{-15} seconds) and close to the measured 320 attoseconds. They also predicted the variation of the observed charge-transfer time with the polarization of the excitation light (see the figure). This effect still waits for experimental verification.

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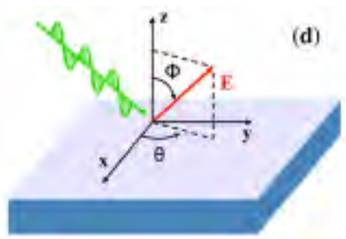

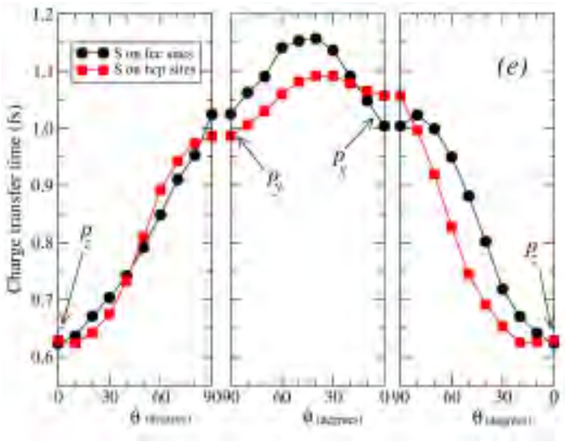

*Figures. Panel (**a**) shows the c(4x2) Ru(0001) surface. Different excitation geometries translate to different initial electronic wavepackets. The initial wavepackets are constructed by projecting linear combinations of the sulphur 3p states onto the relevant energy window. Panels (**b**) and (**c**) show the electron density associated with "pz" and "px" orbitals. Panel (**e**) shows the charge transfer time as a function of the symmetry of the initial wavepacket (i.e. the field polarization in the experiment, see panel (**d**)).*

The calculations were based on state-of-the-art electronic structure calculations, using the so-called density-functional theory, to compute the details of the combined adsorbate-substrate system.

This theoretical method has also been applied to unveil the importance of the elastic contribution to the total widths of the quantum well states at alkali overlayers on Cu(111)[2], allowing to explain the spectra obtained with scanning tunneling spectroscopy (STS) in such surfaces. More recently the case of Ar monolayers on Ru(0001) have been also studied[3], finding again values and trends for the charge-transfer times in good agreement with the core-hole-clock experiments.

Dr. Sánchez-Portal and Prof. Echenique, and their experimental colleagues are treating to extend their results to resolve the different behavior of electrons with different spins in magnetic systems. This can provide crucial information for developing future electronic devices based on the spin of the electrons, a field known as 'spintronics'. Charge-transfer is also key to many biological processes such as photosynthesis. ■

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Potential Energy Landscape of a Simple Model for Strong Liquids

by *A.J. Moreno*[1,2], *F. Sciortino*[2,3], *I. Saika-Voivod*[2], *E. Zaccarelli*[2,3], *E. La Nave*[2,3], *S.V. Buldyrev*[4], *and P. Tartaglia*[2]

We introduce a minimal model exhibiting all the phenomenological features characterizing strong behavior in network-forming liquids. The statistical properties of the potential energy landscape can be computed for the first time with arbitrary precision even in the low temperature limit. A degenerate disordered ground state and non-Gaussian statistics for the distribution of local minima are the landscape signatures of strong liquid behavior. Differences from fragile liquid behavior are attributed to the presence of a discrete energy scale, provided by the particle bonds, and to the intrinsic degeneracy of topologically disordered networks.

In this work we aim to clarify the statistical properties of the PEL of strong liquids.

The structural relaxation time of a supercooled liquid increases over 13 orders of magnitude with decreasing temperature. At some given temperature, equilibration is not possible within laboratory time scales and the system becomes a glass. In 1969, Goldstein proposed to view a supercooled liquid as a point moving in the high-dimensional landscape of its potential energy. At low temperatures the system is located in deep valleys of the potential energy landscape (PEL). Short-time vibrational dynamics correspond to motions within a valley. Long-time structural relaxation occurs via motion between neighbouring valleys separated by high energy barriers.

In the Stillinger-Weber approach, the PEL is partitioned into basins around its local minima. The total entropy is obtained as a sum of a *configurational* contribution, given by the distribution and multiplicity of the local minima, and a *vibrational* contribution, related to the configurational volume available within the basins. Nowadays, the PEL is a key concept in the understanding of the glass transition problem. In particular, numerical investigations provide strong correlations between geometrical properties of the *static* PEL and *dynamic* features of supercooled liquids.

A glass-forming liquid is classified as *fragile* if the temperature dependence of its structural relaxation time on approaching the glass transition shows large deviations from Arrhenius behavior. If no deviations are observed, the liquid is classified as *strong*. Polymeric or low molecular weight organic liquids, where interactions do not show a marked directional character, are fragile. Inorganic liquids forming open network structures are strong.

In this work[1] we aim to clarify the statistical properties of the PEL of strong liquids. We carry out simulations on a system of particles interacting via a spherical hardcore plus a finite square-well potential, with a constraint on the maximum number (four) of bonded neighbours per particle. As a consequence of the finite square-well interaction, particles form a connected network of reversible bonds. The population of broken bonds decreases with decreasing temperature. By construction, the energy of the ground state (the fully bonded network) is unambiguously known. Contrary to simulations in real systems, the ground state can be reached *in equilibrium* and no extrapolations are needed in the calculation of thermodynamic functions at low temperatures.

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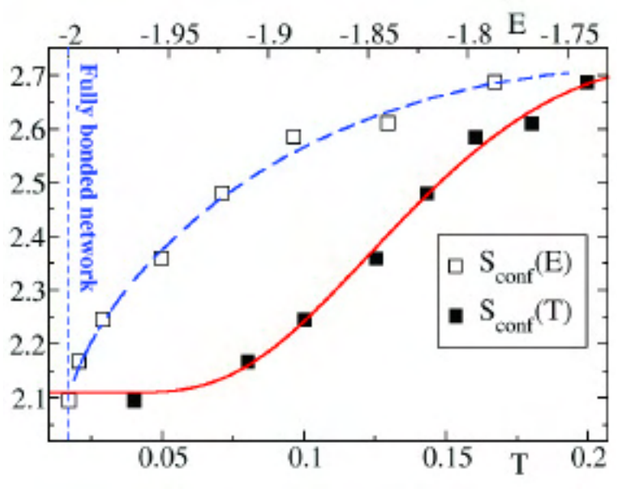
Local minima are identified as topologically different bonding patterns. The basin associated to a given minimum corresponds to the configurational volume that can be explored by deforming the bonding pattern without breaking or forming bonds. With this definition, vibrational and configurational entropies can be formulated for the first time in an exact way, and the accuracy in their numerical evaluation is just limited by the precision of statistical averages.

The universal dynamic features shared by strong liquids, as Arrhenius behavior of the diffusivity, and weak stretching for dynamic correlators, are reproduced by this minimal model. The evaluation of the configurational entropy provides several striking features. In contrast to observations in fragile liquids, the distribution of local minima strongly deviate from Gaussian behavior. This feature is consistent with PEL analysis in atomistic models of silica (the archetype of strong behavior), and originates from the lower energy cut-off and the *discrete* energy scale provided by the inherent network of bonds.

The configurational entropy *per particle* takes a finite value in the limit of low temperature (see figure). This feature is confirmed by displaying the configurational entropy vs. the energy. The fact that the ground state (the fully bonded network) is reached in equilibrium excludes the possibility of ulterior changes in thermodynamic functions. According to this result, strong liquids are characterized by a degenerate ground state, originating from the exponential number of topologically distinct patterns the fully bonded network can adopt.



The configurational entropy per particle takes a finite value in the limit of low temperature.

We like to mention that, in a different physical context, this model provides a way of forming low-density arrested states (gels) without encountering phase separation[2]. Due to the constraint in the maximum number of bonds per particle, energy differences between particles located at the bulk and at the surface of the spanning clusters are strongly reduced, and the phase-separated region is largely shrunk. This result is relevant for gel-forming systems showing localized and directional interactions, as patchy colloids or some proteins. ■

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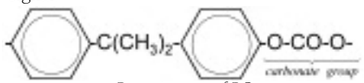
Why is Polycarbonate An Excellent Engineering Polymer?

by *A. Alegría*[1,2], *O. Michelena*[1], *J. Colmenero*[1,2,3]

The molecular origin of the excellent mechanical properties of bisphenol-A polycarbonate has been debated since more than 20 years without any definitive consensus so far. One of the more recent and controversial results on this topic was found when the phenylene ring dynamics was investigated by using neutron scattering. These measurements provided the first experimental confirmation of phenylene ~90° rotation, which was predicted to occur from numerical calculations on the small molecule analogues of polycarbonate. We have shown that this particular molecular motion is of utmost importance on the secondary dielectric relaxation of polycarbonate and being therefore deeply connected with its excellent properties.

It is likely you have realized that plastics are present everywhere in your daily life. You can find these materials in your computer, printer, furniture, car... This is because engineering polymers are durable, light, cheap, and have good mechanical and thermal properties making them suitable for a huge number of applications. Polycarbonate (PC) is one of the most widely used engineering thermoplastics. The interesting ultimate mechanical properties of PC are related to the ability of it to accommodate a stress, which involves highly activated molecular motions including those of the phenylene rings. That is why considerable efforts have been made to identify the molecular origin of the so-called secondary relaxations in PC and other related polymers. Though the existence of these processes and their main general features are established for many decades, their microscopic origin remained elusive. Traditionally these polymers have been studied by mechanical relaxation techniques and nuclear magnetic resonance. Only very recently, a detailed and systematic neutron scattering investigation of the phenylene ring dynamics in engineering thermoplastics, has demonstrated that only in PC, phenylene rings performs ~90º rotations, in addition to the π-flip motions generally observed in this family of polymers. In fact, numerical calculations on the small molecule analogues of polycarbonate already predicted phenylene ~90º rotations to occur.

Thus, taking these results into account, we have revisited the dielectric relaxation behavior of polycarbonate by new careful measurements over extremely broad ranges of both temperatures (50 - 350 K) and frequencies (10mHz-1GHz), looking in very detail for the effects of molecular orientation on the dielectric signal of the sample. The first comparison between the results obtained in the oriented sample with that of unoriented PC revealed a non-uniform reduction of the dielectric losses, the part of the response more reduced by orientation having the dynamic characteristics of the phenylene ~90º rotations as determined from neutron scattering. In addition, a further careful analysis of the dielectric losses of PC has allowed to evidence that the second main contribution to the dielectric relaxation has the same dynamic characteristics than those of phenylene ring π-flips. These results imply that the dielectric relaxation of PC arises from the strong coupling between the phenylene ring motions and those of the carbonate unit (see below), being this latter motion the ultimate responsible of the observed dielectric signal.



Repeating unit of PC

Namely, although the pheylene π-flips should not alter the molecule geometry much because of the high symmetry of the rings, the molecular distortions occurring during the phenylene π-flips would induce significant rearrangements of the surrounding units and particularly of the carbonate group. On the other hand, the calculations on small molecules analogues of PC showed that phenylene ~90º rotations have to be accompanied by similar jumps of the adjacent carbonate units, hence contributing very noticeably to the dielectric relaxation. In addition to these main contributions, the dielectric relaxation of PC presents a weak and faster component that resulted directly connected with small angular oscillations of the phenylene rings. This molecular assignment is illustrated in Figure 1. It allows rationalizing the 'anomalous' behaviors found in the dielectric relaxation of PC:

i) It allows the understanding of why molecular orientation reduces less the slowest component of the dielectric relaxation. The high symmetry corresponding to a phenylene π-flip yields the ring after the π-flip to be at the same position as it was before, and therefore, only short living fluctuations of the environment are necessary. On the other hand, after the phenylene ~90º rotation, the ring needs to have the corresponding available room, which obviously is much more difficult in a sample having molecular orientation, where the rings tend to stack parallel to each other.

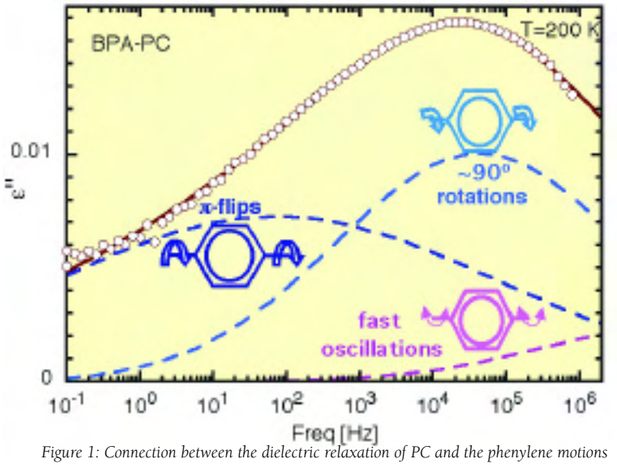


Figure 1: Connection between the dielectric relaxation of PC and the phenylene motions

ii) The same arguments also explain why when decreasing temperature there is a strong reduction of the contribution of phenylene ~90º rotations to the dielectric relaxation. The higher density would strongly diminish the probability of finding long living holes for accommodate a ring after a ~90º rotation. In fact, the marked temperature dependence of the main dielectric contributions makes the shape and average time of the dielectric relaxation to show unusual temperature behavior.

These results lead us to conclude that the phenylene ~90º rotations are of utmost importance in relation to the excellent mechanical properties of PC. This is further supported by the fact that it is just at the ductile-brittle transition temperature where the probability of phenylene ~90º rotations to occur starts increasing rapidly. ■

The interesting ultimate mechanical properties of PC are related to the ability of it to accommodate a stress, which involves highly activated molecular motions including those of the phenylene rings.

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Dynamic Confinement in Miscible Polymer Blends

by *A.-C. Genix[1], M. Tyagi[1], A. Arbe[2], F. Alvarez[2,3], J. Colmenero[1,2,3], L. Willner[4], D. Richter[4], B. Frick[5], J.R. Stewart[5]*

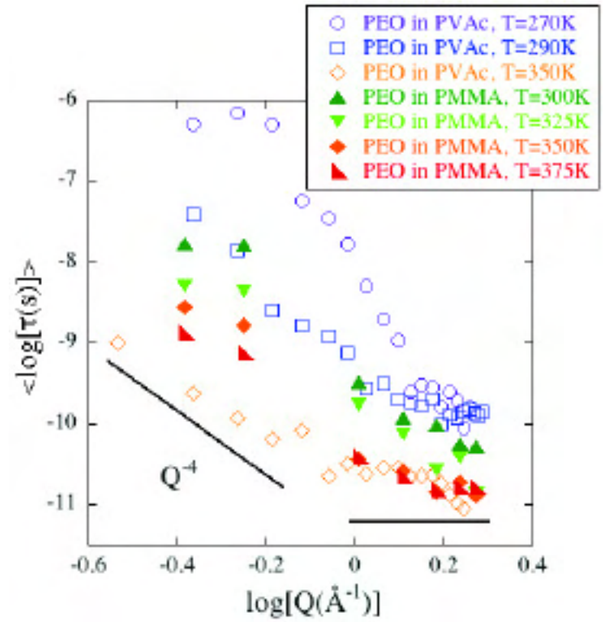
Neutron scattering measurements with space/time resolution have provided first direct experimental evidence at a molecular level of confinement effects in a miscible polymer blend. These are induced by the freezing of the component with higher glass transition temperature T_g and are a direct consequence of the dynamic heterogeneity characteristic of polymer mixtures. Fast localized dynamics are observed for the low-T_g component, with associated jump lengths of about 2-3Å. These results have been corroborated by complementary fully atomistic molecular dynamics simulations.

Extreme dynamic heterogeneity in diluted blends leads to confinement effects with enhanced local dynamics in the glassy state.

By now the dynamic heterogeneity is a well established feature of polymer blends. It refers to the observation, even in a thermodynamically miscible system, of two different characteristic timescales for segmental relaxation, each of them corresponding to each component. A large experimental effort has been devoted to the phenomenological characterization of this property and nowadays models based on the concept of self-concentration successfully capture the main ingredient leading to two distinct timescales. Dynamic heterogeneity is magnified in highly asymmetric blends. This asymmetry can refer to the blend composition (diluted in one component) or also to the dynamics of the pure polymers (very different glass-transition temperatures, T_g). Thus, an intriguing question arises: what happens under such extreme conditions that, as a consequence of the strong dynamic heterogeneity, the slow component is completely frozen on the timescale of the segmental motions of the fast component?

First experimental evidences of a non-equilibrium situation were reported from dielectric spectroscopy studies for poly(vinyl methyl ether) (PVME) in blends with high concentration of polystyrene (PS). The behavior found, strongly, suggested the emergence of confinement effects for the fast component (PVME) when PS approaches its glass transition in the blend. However, dielectric spectroscopy does not provide the spatial information necessary to fully characterize the dynamics of the fast component. The required space/time resolution at a molecular level is offered by neutron scattering techniques, which allow in addition the selective study of one of the blend components by deuteration of the other polymer chains.

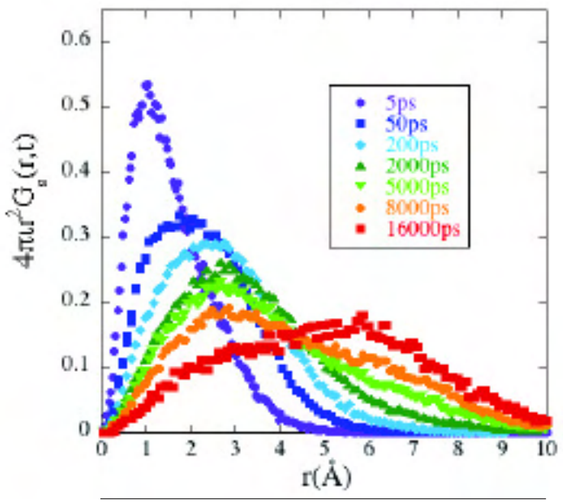
Direct microscopic observation of the confined dynamics was realized by neutron scattering on poly(ethylene oxide) (PEO) in blends with poly(methyl methacrylate) (PMMA) and poly(vinyl acetate) (PVAc) with low concentrations of PEO. The T_gs of the homopolymers differ by almost 200K (PEO/PMMA) and 100K (PEO/PVAc). In the high momentum transfer (Q) region, the characteristic times obtained for PEO in both mixtures clearly deviate from the expected momentum transfer dependence in the melt (Q^{-4}) and become nearly constant, suggesting the occurrence of localized motions (see Figure 1). From the Q-range where this flattening is observed, a spatial length scale of about 2 Å could be deduced for such hopping processes. Moreover, we note that in the low-Q regime, for the lowest temperatures investigated (below the T_g of the slower component) the Q-dependence is much steeper than that corresponding to Rouse dynamics. This would imply that the large-scale motions are clearly slowed down with respect to the equilibrium behavior, and could be considered as a signature of the freezing of the global chain dynamics as a consequence of the confinement of PEO motions by the rigid matrix formed by the other component in the blend.



Momentum transfer dependence of the timescales obtained by neutron scattering for PEO in blends with PMMA and PVAc

In a complementary way, molecular dynamics simulations were performed in the blend PEO/PMMA with 10% PEO content. As can be seen in Figure 2, the occurrence of jumps in PEO is supported by the simulation results, which allow direct insight in real space. The development of a second maximum in this function reveals hopping processes with associated jump lengths of the order of 3 Å (see the distance between the two maxima for the longest time), in very good agreement with the neutron scattering results.

Thus, we have observed and characterized the confined motions taking place in a polymer surrounded by other rigid chains. The plasticization induced by blending, together with the emergence of such confinement effects leading to a fast local dynamical process, might provide a new route to tailor the properties of new commodities based on already existing materials. ■



Radial self-correlation function obtained from the MD-simulations for PEO in the PMMA-blend at different times

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Polybutadiene Dynamics Close to the Glass Transition: Hop, hop! We're freezing!

by *J. Colmenero[1,2,3], A. Arbe[2], F. Alvarez[1,2], A. Narros[1], M. Monkenbusch[4], D. Richter[4]*

The potential of (carefully validated) fully atomistic MD-simulations is demonstrated by unravelling the puzzling situation concerning the dynamics of polybutadiene close to the glass transition. The identification in real space of hopping processes has put into a context the variety of experimental observations for this polymer. This was only possible by selective scrutiny of the different atomic species. Though linked through chain connectivity, polybutadiene hydrogens located in the different structural units preserve their own dynamical identities close to the glass transition.

The controversial results from experiments close to the glass transition reflect the rich local dynamics at microscopic level.

Many original works in polymer physics have been performed on the "in principle" simple and archetypal polybutadiene, -[CH_2-CH=CH-CH_2-]$_n$. In particular, this was the favorite sample for neutron scattering experiments during many years, yielding quite a number of relevant observations, mainly by neutron spin echo (NSE). For instance, it was the first polymer where NSE measurements at the first structure factor peak revealed the structural (α) relaxation. Later, during a pioneering NSE excursion in the intramolecular region, an additional process was found, that was active in the neighborhood of the glass transition (T_g = 178 K). The nearly identical temperature dependencies of the dielectric β-relaxation and the dynamic structure factor at the second peak (intrachain) suggested a common molecular origin for both processes. However, a difference of more than two orders of magnitude in the associated characteristic timescales prevented a definitive connection between them (see Figure 1). In the mean time, the relaxation map of polybutadiene has become even more puzzling, since two additional processes were reported from light scattering experiments (see Figure 1).

Trying to shed some light in the molecular origin of all these processes, we have performed fully atomistic MD-simulations on this system at 200 K. Our cubic cell contained one chain of 130 monomers with a microstructure (39 % cis; 53 % trans; 8 % vinyl units) similar to that of the real sample. Two big advantages of fully MD-simulations are: (i) to easily allow monitoring different atomic species and (ii) to directly access the real space. We have exploited both in this work and an example of the outcome is shown in Figure 2. First of all, we realize that the main feature of the hydrogen motions at timescales close to the nanosecond is the predominance of localized processes —the radial distribution functions develop a more or less evident second maximum at about 2.7 Å. It is worth noting that this feature is hidden in the reciprocal space accessed by the experiments. The second observation is the markedly heterogeneous behavior: each kind of hydrogen evolves in a different way! The most diverse motions seem to be carried out by the hydrogens attached to the double bonds in the cis and trans units (see the insert of Figure 2).

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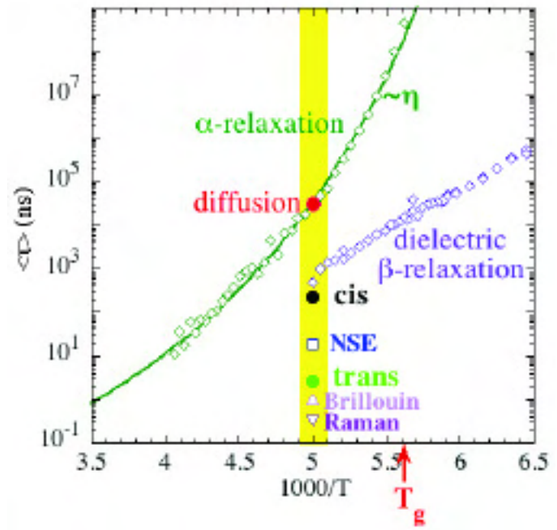
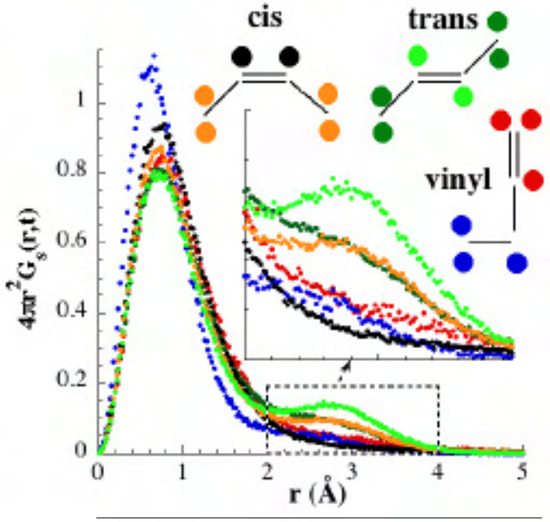
The real space data of these two species were fitted by considering simultaneous occurrence of hopping processes and sublinear diffusion due to the structural relaxation. We obtained the following results: The trans hydrogens undergo jumps of a well defined length, 2.5 Å, while the cis hydrogens show jump distances broadly distributed around the same value. For both kinds of atoms we obtained broad distributions of characteristic times that can be attributed to the inherent disorder in our polymer. Interestingly, the average timescale observed for the cis atoms is much longer than that characterizing the trans motions. They have been displayed in Figure 1. The comparison with previous experimental results is revealing: (i) the fastest motions of the trans units are probably responsible for the light scattering observations; (ii) the dielectric β-relaxation is produced by the localized motions carried out by the cis group —very plausible, since the dipole moment in polybutadiene is associated to this unit—; and (iii) NSE delivers an average of both motions. This is also logical, since the dynamic structure factor relates to all atoms in the sample, carbons and deuterons, and therefore an intermediate timescale is observed. Thus, the controversial polybutadiene experimental observations are just the result of rich local dynamics at microscopic level. Finally, concerning the subdiffusive component of the motions, we found a perfect agreement with the expectation for the contribution of the α-relaxation (see Figure 1), strongly supporting the consistency of the framework and the analysis of the data. ■



Variety of timescales identified for polybutadiene by different experimental methods (empty symbols) and the processes observed by the simulations (full dots).



Radial self-correlation function at t = 1 ns obtained from the MD-simulations for the different hydrogens in polybutadiene (the colors indicate for which atom).

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The Surroundings Really Matter... Also for Polymer Motion

by *D. Cangialosi[1], G.A. Schwartz[1], A. Alegría[2,3], J. Colmenero[1,2,3]*

The segmental dynamics of a polymer, giving rise to the glass transition, is generally altered when this polymer is mixed to another one with different mobility. This is mainly due to the fact the polymer "senses" the local environment around it up to a scale of several nanometres. Thus, the characteristic volume involved in the motion will possess an effective concentration in this component that is higher than the bulk concentration of the blend. This picture can be successfully incorporated in one of the available theoretical approaches describing the dynamics of glass-formers: the Adam-Gibbs theory relating the mobility to the number of available configurations.

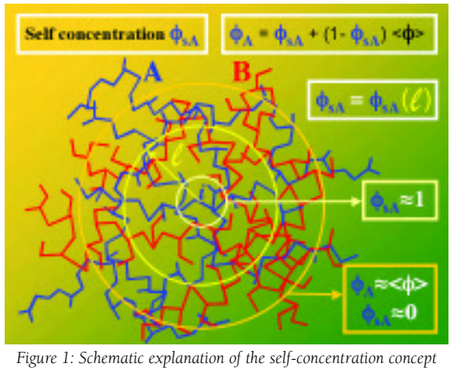

Figure 1: Schematic explanation of the self-concentration concept

The last decades have seen a growing interest in the study of miscible polymer blends due to the potential application of these systems. Furthermore, the study of the segmental dynamics of these systems offers the possibility of extracting fundamental information on the nature of the glass transition.

The main feature of the dynamics of polymer blends is the speed-up or slow-down of the dynamics of one polymer, when this is surrounded by another polymer with relatively different dynamics. The effect of the other component of the blend is strongly related to the length scale involved in the dynamics. The characteristic length scale determines the effective concentration experienced by a given polymer segment. This feature, which is known as self-concentration effect, is moreover enhanced by chain connectivity. The essential features of this concept are explained in Figure 1 and can be summarised as follows: when a volume is centred on the basic structural unit of one of the polymers of the blend, the effective concentration will be different from the macroscopic one. Two extremes cases are possible: i) if this volume equals the volume of the basic structural unit, then the effective concentration is one, and ii) if, on the other hand, this volume is large enough, then the effective concentration equals the macroscopic one.

To rationalize the effect of blending on the dynamics of polymers, we have proposed a model based on the combination of the self-concentration concept with the Adam-Gibbs (AG) theory, relating the characteristic time for the segmental relaxation with the number of configuration the system can explore. This

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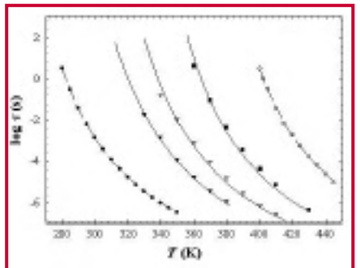

Figure 2: Logarithm of the relaxation time vs. temperature for pure PoClS (open circles), PS700 (filled circles) and for PoClS in blends with PS700 with weight percentages: 25% (filled triangles), 50% (open triangles) and 75% (filled squares). The solid lines are the fittings of the model to the blends experimental data.

number, namely the configurational entropy, can be obtained from calorimetric measurements. Furthermore, we have exploited the concept of a growing length scale with decreasing temperature implicit in the AG theory that proposes a correlation between the configurational entropy and the characteristic length scale, such that at high temperatures the characteristic volume is small but it increases as temperature is reduced. The model relies on just one fitting parameter, namely the proportionality constant between the length scale and the configurational entropy, which is unreliably determined from the AG theory. As this parameter is polymer specific, one can predict the dynamics of miscible polymer blends once this parameter has been determined studying the dynamics of other polymer blends as well as polymer-solvent mixtures. To sum up, once the only unknown parameter of the model is obtained indirectly, the dynamics of miscible polymer blends can be fully predicted starting from the knowledge of the dynamics and the thermodynamics of the pure components of the blend.

We have obtained these results by measuring the segmental dynamics of several miscible polymer blends and of the pure components of the blends. This was done employing broadband dielectric spectroscopy (BDS), which is capable of measuring selectively the mobility of all those systems possessing relaxing dipoles. Moreover, precise determination of the specific heat of the pure components of the blends has been performed by modulated differential scanning calorimetry (MDSC). This allowed evaluating the configurational entropy of the pure components of the blend as required by the model.

As an example, we show in Figure 2 the segmental dynamics of poly-o-chlorostyrene (PoClS) in polystyrene oligomer (M_n=700 g/mol) (PS700). The two polymers display a rather large dynamic contrast being the glass transition temperature (T_g) of PoClS equal to 402K and that of PS700 equal to 280K. Moreover, PoClS possesses a far larger dipole moment than PS700 and, therefore, the dielectric response can be attributed to the segmental relaxation of PoClS in the blend. From inspection of Figure 2, we clearly observe that the dynamics of PoClS is accelerated by the presence of the more mobile PS700. The acceleration is enhanced for blend with larger PS700 content. These qualitative results are a clear indication that the surrounding plays a decisive role in affecting the dynamics of polymers. These features are quantitatively captured by our model as indicated by the solid lines in Figure 2.

Our results also indicate a prominent role of self-concentration and provide an estimation of the length scale involved in the segmental relaxation of polymer blends. This is universally found to be between 1 and 3 nanometers. ■

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Once the only unknown parameter of the model is obtained indirectly, the dynamics of miscible polymer blends can be fully predicted starting from the knowledge of the dynamics and the thermodynamics of the pure components of the blend.

Water and Polymers: A New Route to Approach the Dynamics of Biological Water

by *S. Cerveny*[1], *J. Colmenero*[1,2,3], *A. Alegría*[2,3]

Water is a substance that fascinates everyone, newborn babies or scientists alike, and it is essential for all life on earth. However, despite its importance and widespread interest we do not fully understand the dynamic behavior of water in confining environments, as it is the case of biological systems. In this work we face this problem by studying water dynamics in mixtures with water-soluble synthetic polymers. The results give new insight on the dynamics of confined water in more complex environments such as biological materials.

Biological macromolecules —proteins and DNA— are physiologically inactive without water.

While many aspects of structure and dynamics of bulk water can be regarded as reasonably understood at present, the same is not true for the water which is found in interfacial or restricted environments, such as the surface of proteins or micelles. Water at the surface of a protein defines a molecular layer that has been termed "biological water" or "first hydration shell" and exhibits unique characteristics. In addition, there is a second hydration shell formed by loosely bounded water molecules. However, biological systems are extremely complex since movements of the host materials mask and can directly affect the water dynamics. Contrarily, synthetic polymers (such as poly (vinyl methyl ether)) offer the possibility to study the water dynamics in a well controlled environment since the polymeric chains often remain frozen in the temperature range where the water dynamics is relevant and the presence of the polymer acts as inhibitor of crystallization.

We have investigated the properties of PVME/H_2O mixtures by both dielectric and calorimetric methods. Our experiments have been focused on the water dynamics in the low temperature range (150-200 K) where the PVME matrix remains essentially immobile since the glass transition temperature (T_g) of dry PVME is around $T_g \approx 250$K. We considered the hydration water dynamics at several polymer concentrations (from concentrated solution up to 50 wt%). In addition, dielectric relaxation spectroscopy is suited for the investigation of the H-bond rearrangement dynamic due its ability to monitor the motion of water dipole.

Our recent work confirms that different hydration shells can be also found in hydrated polymers at low temperatures. In the case of PVME-water mixtures, at water content lower than 34 wt%, water molecules interact strongly with the polymer matrix, which suppress its translational motions and limit their reorientation ability (first hydration shell). This is notice for both the impossibility of crystallization and a dielectric relaxation weaker than that expected from water molecules without orientational restrictions (Figure 1).

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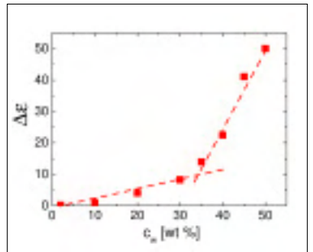

Figure 1: Dielectric relaxation strength of PVME aqueous solutions for water concentration up to 50% wt. A non-monotonous increase with water content is found defining clearly when water molecules start forming the second hydration layer.

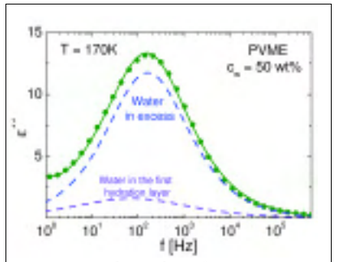

Figure 2: Dielectric loss of a PVME-water solution (c_W=50 wt%). Note the decomposition of the total dielectric signal (solid line) in a contribution attributed to the first hydration shell water molecules (dotted line) and another from loosely bounded water (dashed line).

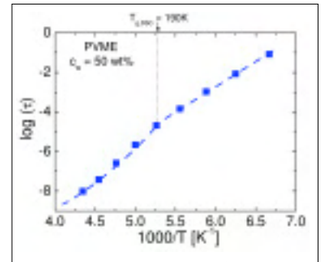

Figure 3: Relaxation time of a PVME-water solution (c_W=50 wt%). Note the crossover between Arrhenius and VFT behavior at $T_{g,DSC}$.

In contrast, at high water concentration all the hydrophilic sites are already occupied and, therefore, there are water molecules which are surrounded only by other water molecules. This excess water behaves more like-bulk water: it tends to crystallize easily and has a stronger contribution to the dielectric relaxation reflecting weaker restrictions for reorientations. Thus, the measured dielectric signal can be modelled as a sum of two different contributions: one related with the water molecules H-bonded to the polymer (or water in the first hydration shell and obtainable from the spectra with c_W=30 wt%) and the other one related to the water in excess or water in second hydration level (Figure 2).

Another interesting feature of water dynamics is that it shows an Arrhenius temperature dependence at the low temperatures, where the polymer matrix remains frozen, and crosses-over to the behavior typical of glass formers above this temperature (Figure 3).

Finally, it is important to note that the feature showed for PVME is also valid for other water soluble polymers [such as poly(vinyl pyrrolidone)] and for small molecules (such as ethylene glycol or propylene glycol and its oligomers). ■

Our recent work confirms that different hydration shells can be also found in hydrated polymers at low temperatures.

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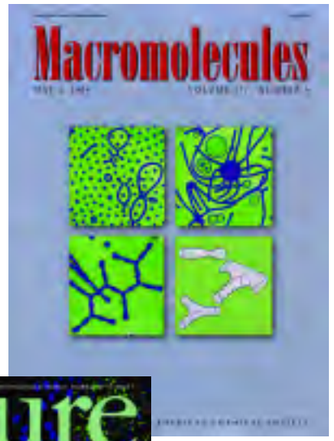

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A.J. Garcia-Adeva, R. Balda, J. Fernandez, E.E. Nyein, and U. Hommerich.
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B. Gumhalter.
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J.E. Ortega, M. Ruiz-Oses, and J. Kuntze.
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Lifetimes of Shockley electrons and holes at Cu(111).
M.G. Vergniory, J.M. Pitarke, and S. Crampin.
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S. Kurth, G. Stefanucci, C.O. Almbladh, A. Rubio, and E.K.U. Gross.
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F.J. García de Abajo, G. Gómez-Medina, and J.J. Sáenz.
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Dynamics of poly(ethylene oxide) in a blend with poly(methyl methacrylate): A quasielastic neutron scattering and molecular dynamics simulations study.
A.C. Genix , A. Arbe, F. Alvarez, J. Colmenero, L. Willner, and D. Richter.
Physical Review E **72**, 031808 (2005).

Fermi gap stabilization of an incommensurate two-dimensional superstructure.
F. Schiller, J. Cordón, D. Vyalikh, A. Rubio, and J.E. Ortega.
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M. Palummo, O. Pulci, R. Del Sole, A. Marini, M. Schwitters, S.R. Haines, K.H. Williams, D.S. Martin, P. Weightman, and J.E. Butler.
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S.H. Chong, A.J. Moreno, F. Sciortino, and W. Kob.
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E. Zaccarelli, S.V. Buldyrev, E. La Nave, A.J. Moreno, I. Saika-Voivod, F. Sciortino, and P. Tartaglia.
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F. Schiller, M. Ruiz-Osés, J. Cordón, and J.E. Ortega.
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F.J. García de Abajo, G. Gómez-Santos, L.A. Blanco, A.G. Borisov, and S.V. Shabanov.
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T. Brixner, F.J. García de Abajo, J. Schneider, and W. Pfeiffer.
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F. Schiller, R. Keyling, E.V. Chulkov and J.E. Ortega.
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Energy landscape of a simple model for strong liquids.
A.J. Moreno, S.V. Buldyrev, E. La Nave, I. Saika-Voivod, F. Sciortino, P. Tartaglia, and E. Zaccarelli.
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C. Corriol, V.M Silkin, D. Sánchez-Portal, A. Arnau, E.V. Chulkov, P.M. Echenique, T. von Hofe, J. Kliewer, J. Króger, and R. Berndt.
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J. Hager, R. Matzdorf , J. He, R. Jin, D. Mandrus , M.A. Cazalilla, and W.E. Plummer.
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Two-component fermi gas on internal-state-dependent optical lattices.
M.A. Cazalilla, A.F. Ho, and T. Giamarchi.
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Electromagnetic Surface Modes in Structured Perfect-Conductor Surfaces.
F.J. García de Abajo and J.J. Sáenz.
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Anderson localization in carbon nanotubes: defect density and temperature effects.
B. Biel, F.J. Garcia-Vidal, A. Rubio, and F. Flores.
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I.A. Howard, G.G.N. Angilella, N.H. March, and C. Van Alsenoy.
Physics and Chemistry of Liquids **43**, 441 (2005).

Interacting inhomogeneous electron liquids with harmonic confinement: s-wave model.
I.A. Howard and N.H. March.
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Fingerprints of quantal Wigner solid-like correlations in D-dimensional assemblies.
N.H. March and R.H. Squire.
Physics Letters A **346**, 355 (2005).

Total resonant absorption of light by plasmons on the nanoporous surface of a metal.
T.V. Teperik, V.V. Popov, and F.J. García de Abajo.
Physics of the Solid State **47**, 178 (2005).

Diffusional and vibrational properties of Cu (001)–c(2x2)–Pd surface alloys.
S.V. Eremeev, G.G. Rusina, I.Yu. Sklyadneva, S.D. Borisova, and E. V. Chulkov.
Physics of the Solid State **47**, 4, 758 (2005).

Neutron Scattering Investigations on Methyl Group Dynamics in Polymers.
J. Colmenero, A.J. Moreno, and A. Alegría.
Progress in Polymer Science **30**, 1147 (2005).

A viable way to tailor carbon nanomaterials by irradiation induced transformations.
R. Caudillo , H.E. Troiani, M. Miki-Yoshida, M.A.L. Marques, A. Rubio, and M.J. Yacamán.
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A.K. Kazansky, A.G. Borisov, and J.P. Gauyacq.
Surface Science **577**, 47 (2005).

Induced charge-density oscilations at metal surfaces.
V.M. Silkin, I.A. Nechaev, E.V. Chulkov, and P.M. Echenique,
Surface Science **588**, L239 (2005).

Electron-phonon coupling and lifetimes of excited surface states.
B. Hellsing, A. Eiguren, E.V. Chulkov, and P.M. Echenique.
Surface Science **593**, 12 (2005).

OUR RESEARCHERS

DIPC hosts long-term researchers that collaborate with visiting researchers on leading topics.

Fellows Gipuzkoa

Dr. A. Moreno
University of Roma La Sapienza, Italy
01-01-2005
Investigation by means of molecular dynamics and Monte Carlo simulations of:
· Energy landscape and non-ergodic transitions in supercooled liquids
· Dynamics of linear molecules in disordered static environments
· Dynamic heterogeneities in polymer blends

Dr. V. Silkin
Russian Academy of Science, Tomsk, Russia
03-01-2002
· Surface science
· Electronic excitations at the metal surfaces
· Electron dynamics in metals, metal surfaces and systems with reduced dimensionality

Dr. M.A. Cazalilla
ICTP Trieste, Italy
01-01-2003
· Strongly correlated systems, Bose Condensates, Mesoscopic and low-dimensional systems in and out of equilibrium
· Electronic excitations in surfaces and anisotropic systems

Dr. M. Alducin
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-09-2003
· Lifetime of low energy electrons in paramagnetic materials: spin effects and non-linear effects
· Interaction of atoms/ions with surfaces: charge exchange and energy loss
· Dielectric response of covered metal surfaces

Dr. J. Aizpurua Iriazabal
National Institute of Standards and Technology (NIST), USA
01-01-2004
Electronic and optical properties of metal nanostructures and semiconductor low-dimensional systems.
Nanooptics is a rapidly emerging branch of optics driven by the goal to control, manipulate and probe with light on the nanoscale. Simulating nanoscale optical microscopy and spectroscopy is challenging due to the need to describe light fields from the near-field to the far-field, to determine the influence of the probe, and to identify any contribution of the local environment. Metal nanostructures will be extensively studied to develop uses in key applications such as field-enhanced spectroscopies, near-field scanning optical microscopy (NSOM), or single molecule spectroscopy. Parallel to this effort, the electronic and optical properties of low-dimensional semiconductor systems will be studied with special emphasis on the study of heterostructures of quantum wires and quantum dots with applications to quantum computing with entangled states, or spin polarized photon generation.

What is Fellows Gipuzkoa?

Thanks to the support and financing of the Provincial Authority of Gipuzkoa, DIPC has been able to set up Fellows Gipuzkoa; a program which allows young scientists, mostly from the Basque Country, who have been working abroad, to return. DIPC acts as a "landing platform" by means of a five year contract. For more information, visit http://dipc.ehu.es.

Post-doctoral Positions

Dr. J. Sacristán
Instituto de Ciencia y Tecnología de Polímeros, CSIC, Madrid, Spain
01-04-2002 through 31-03-2005
My research focuses on the application molecular dynamics methods to study the structure and properties of a variety of polymer on the atomic scale. We are interested in bulk, free and confined polymer systems, glass transition in polymer films, static and dynamic properties of thin polymer films.

Dr. A. Ayuela
Helsinki Technical University, Finland
14-05-2003
· Ab-initio studies of magnetism with dimensionality (magnetic anisotropy, spin spirals, Curie temperature...): nanowires, multilayers, magnetic shape memory alloys
· Phase field and ising description of magnetic phenomena

Dr. F. Schiller
Universität Dresden, Germany
01-10-2003 through 31-08-2005
Crystalline and electronic structure of thin Be and Mg films.

Dr. M. Grüning
VRYJE Universiteit, Amsterdam, The Netherlands
15-11-2003 through 31-12-2005
Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

Dr. C. Corriol
University of Liverpool, UK
01-01-2004 through 31-12-2005
Using first-principle calculations applied to STM image simulations, we want to understand the influence of the tunneling resistance and of the coverage on the aspect of the simulated and experimental images for adsorbate-covered systems as O/Ru(0001). In doing so, we try to unravel the intricate interplay between electronic effects and surface geometry. The inclusion of forces between sample atoms and tip atoms is also an objective of our work. Finally, we are involved in tunneling spectra calculations.

Dr. I. Nechaev
Statal University of Tomsk, Russia
10-02-2004
Electron excitations in ferromagnetic materials.

Dr. S. Cerveny
Chalmers University of Technology, Sweden
01-03-2004
General framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other experimental techniques and MD-simulations.

Dr. G. Schwartz
Chalmers University of Technology, Sweden
01-03-2004
General framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other experimental techniques and MD-simulations.

Dr. D. Cangialosi
University of Delft, Holland
01-03-2004
Positron annihilation lifetime spectroscopy to study the dynamics of policarbonate far below Tg.

Dr. M. Tyagi
Jawaharlal Nehru University, India
04-03-2004
The general framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other techniques as, for instance, quasielastic neutron scattering and MD-simulations as well.

Dr. R. Gómez-Medina
Universidad Autónoma de Madrid, Spain
27-09-2004 through 31-12-2005
Calculate photon emission probabilities upon electron bombardment in various metallic nanostructures. This will be compared with recent experimental results form Prof. N. Yamamoto in order to develop a systematies to map plasmon-mode spatial distributions in complex geometries by means of light emission measurements using scanning transmission electron microscopes.

Dr. R. Gaudoin
Rutgers University, New Jersey, USA
15-11-2004
An important issue in many-body and density-functional theory is to understand not only whether the LDA works for a strongly inhomogeneous electron gas, but also to understand whether the nonlocal xc kernel f_xc of an inhomogeneous electron gas can be built from the corresponsding nonlocal xc kernel f_xc of a homogeneous electron gas, a question which was raised by Kohn and Krotscheck many years ago [Phys. Rev. Lett. 57, 862 (1986)] but which has not been solved so far. In order to investigate this issue, we plan to

carry out VMC and DMC calculations of the jellium surface. The idea is to analyze the total and/or surface correlation energy of a jellium slab of a given thickness into contributions from dynamical density fluctuations of various two-dimensional wave vectors. The key point here is that we know the answer in the long wavelength limit, which is the RPA, and we know the answer in the short wavelength limit, which is the LDA. The main ingredient of this analysis is the 2D Fourier transform of the xc-hole density, which one can calculate either from the knowledge of the density-response function (RPA or TDDFT) (see Phys. Rev. B67, 045101 (2003)] or from the knowledge of the many-body wave function (VMC or DMC) by integrating over the coupling constant. It is the VMC and DMC calculation the starting point of the present project.

Dr. A.C. Genix

Laboratoire de Recherche sur les Polymères, Thiais Université Paris XII, France
01-12-2004
Effect of blending on the dynamics of a given polymer. In particular, the system poly(ethylene oxide) / poly(methyl methacrylate) has been chosen, due to the huge difference in the glass transition temperatures of the two components. A combination of quasielastic neutron scattering and fully atomistic molecular dynamics simulations is used to address the question of the dynamic miscibility in this system.

Dr. S. Arrese-Igor

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-01 through 06-04-2005
Sub-Tg molecular motions in engineering thermoplastics.

Dr. M.J. Cabrera San Félix

University of Liverpool, United Kingdom
01-04-2005
Molecular Modelling of water ice in atmospheric and astrophysical environments.

Temporary Contract Positions

Dr. V. Zhukov

Ural Branch of Russian Academy of Sciences, Ekaterunbourg, Russia
01-11-2005
Basing on the LMTO band-structure approach, was developed a first-principle GW+T method of the excited electrons lifetimes calculations. Method combines the evaluation of the lowest term of self-energy within GW approach with the calculations of the highest terms within T-matrix approach. The method has been applied to analyze experimental data for Fe and Ni.
The role of non-spin-flip contributions, Stoner and magnon contribution to the lifetimes and line-widths of excited electrons have been evaluated.

Dr. I. Sklyadneva

Russian Academy of Sciences, Tomsk, Russia
14-05-2003 through 14-05-2006
Surface phonos and electron-phonon interactions in bulk metals and at metal surfaces. Electron-phonon interactions are of paramount importance for the correct description of the temperature dependence of quasiparticle dynamics in bulk metals and at metals surfaces. The goal of the present project is calculations of electron-phonon interactions for overlayers of alkali metals on simple and noble metal surfaces. These calculations will be also done for superconducting materials like MgB2 and for semimetals.

PhD Fellowships

R. Vincent
Université Paul Sabatier, Toulouse, France
01-11-2003
Charge state dependence of the kinetic electron emission induced by slow ions in ferromagnetic metals. In recent experiments in which the spin polarization of electrons emitted when Nitrogen ions interact with a magnetic Fe(100) surface, it has been found that the spin polarization of the electron increases with the charge state of the projectile [1]. In this project we will try to give an explanation for this effect. With this aim, we will use DFT to study the screening characteristics of N ions in a spin-polarized electron gas. Different charge states will be described by introducing holes in the bound Kohn-Sham orbitals. Special attention will be paid to the spin-dependence of the induced density and potential. The scattering of electrons by this spin-dependent potential will be studied in order to characterize the spin dependence of the electronic excitation induced by the slowly moving ion.

R. Pérez Aparicio
Universidad de Valladolid, Spain
15-11-2003 through 31-08-2005
The PhD of Roberto Perez will be focused on the investigation of the dynamics in miscible polymer blends. The main controversial question is whether there exists a relevant length scale beyond which the dynamics of both components in a thermodynamically miscible blend are indistinguishable. In particular, emphasis will be made on the determination of the role played by the concept of "self-concentration" in the different dynamical processes taking place at different length scales in the system. To unravel these problems, neutron scattering techniques offering space-time resolution will be combined with fully atomistic molecular dynamics simulations. Different blend systems will be considered for experiments and simulations.

I. Romero Pérez
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-12-2003 through 31-08-2005
From a theoretical point of view, the electromagnetic response of different metamaterials formed by a periodic distribution of complex objects whose size is much smaller than the wavelength under consideration. These materials will behave like homogeneous media that will be described by their effective dielectric function and magnetic permeability. In particular, left-handed media belong to this class of materials. The main purpose of this work is to extract rules on how to construct metamaterials with on-demand optical properties, and in particular, artificial media that can substain electric and magnetic resonances over a wide range of wavelengths.

M. Martínez Canales
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-10-2004 through 30-09-2005
Metallization and superconducting properties of hydrogen rich alloys at high pressure.

I. Iradi Leiceaga
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-11-2004
Study of polystyrene: Molecular dynamics simulations and neutron scatttering.

M. Massot Pérez
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-12-2004 through 15-05-2005
Electron energy loss spectroscopy and electronic excitations in nanostructures.

A. Sarasola Iñíguez
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-12-2004 through 31-10-2005
Local density approximation in the study of energy loss problems in ion/atom and ion/surface problems.

O. Michelena González
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-01 through 31-05-2005
Study of the effects of thermo-mechanical treatments on Dielectric Secondary Relaxations of engineering thermoplastics.

D. Fernández Pérez
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-01 through 31-07-2005
Methyl group dynamics in disordered systems: Polysulfone, Polycarbonate, Phenoxy and PMMA; a 2H-NMR study.

I. Quintana Fernández
Universidad de Cantabria, Spain
01-01-2005
The aim of the work is to find the relation between the molecular motions and the transport properties in a polymer membrane. By means of quasielastic neutron scattering, we study the molecular dynamics in a polymer membrane: polyethersulfone.

S. Capponi
University of Perugia, Italy
23-10-2005
Dynamics of DNA and proteins by neutron scattering.

VISITING RESEARCHERS

DIPC understands that modern science entails the constant exchange of knowledge and experience to the benefit of all involved.

Long Visits

Prof. W. Schattke
Universität Kiel, Germany
18-01 through 18-04-2005
Variational Quantum Monte Carlo calculations of the electronic properties of solids and surfaces. Theory of Photoemission in semiconductors and metals.

Dr. Y. Koroteev
University Estatal de Tomsk, Russia
04-02 through 01-05-2005
First principles calculations of electronic structure and quasiparticle lifetimes in metals.

Prof. B. Gumhalter
University of Zagreb, Croatia
28-02 through 01-04-2005
Ultrafast electron dynamics on metal surfaces.

Dr. W.A. Hofer
University of Liverpool, UK
29-04 through 30-05-2005
Theory of scanning tunneling microscopy.

Dr. S. Borisova
Physics and Materials Science, Russian Academy of Sciences, Tomsk, Russia
11-05 through 07-07-2005
Phonons in metal adlayers.

Dr. S. Eremev
Institute of Strength Physics and Materials Sciences, Tomsk, Russia
11-05 through 07-07-2005
Phonons and electron-phonon coupling in quantum-well states of adlayers on metals.

Doctorand M.L. Viana Alvarenga
Universidade Federal de Minas Gerais, Brasil
02-06 through 10-08-2005
Genetic algorithms applied to the optimization of surface structures in photoelectron diffraction.

Prof. J. Alonso
Universidad de Valladolid, Spain
18-06 through 15-09-2005
Computational simulation of the intercalation of alkaline atoms in graphite and carbon nanotubes.
Laser induced fragmentation of atomic clusters.

Prof. R. Quirk
The University of Akrom, USA
08-07 through 31-12-2005
Synthesis of functional polymers.

Prof. E. Artacho
University of Cambridge, UK
17-07 through 07-09-2005
- Electronic stopping power in insulators.
- LDA+U, SIC, exact-exchange in DFT calculations.

Dr. C. Lemell
Technische Universität Wien, Austria
19-07 through 30-09-2005
Kinetic electron emission from magnetized surfaces.

Dr. G. Rusina
Russian Academy of Sciences, Tomsk, Russia
02-08 through 30-09-2005
Surface phonons in CuPd surface alloyes.

Dr. T. Teperik
Russian Academy of Sciences, Saratov, Russia
10-08 through 30-09-2005
- Electromagnetic optics.
- Collective resonances in nanostructures.

Dr. S. Cruz Jiménez
Universidad Autónoma Metropolitana-Iztapalapa, México
03-09 through 08-10-2005
Stopping power theory: Study of chemical binding effects on the stopping power of ions in compound target materials as well as development of theoretical models to account for target pressure effects on the stopping and range of heavy ions.
Boxed-in atoms and molecules: Study of spatial confinement effects on the energy levels of atoms/molecules as well as the effect of pressure on molecular conformation and bond compressibility.

Dr. A.Y. Borissov
Université Paris-Sud, France
01-10 through 30-11-2005
Time-dependent density functional theory and wave packet propagation methods.

Doctorand P. Lazic
Rudker Boskovic Institute, Zagrev, Croatia
01-10 through 22-12-2005
Ultrafast electron dynamics on metal surfaces.

Doctorand J. Ramiro Manjarrés
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-10 through 31-12-2005
Relationship between the quality level reached in "hot-embossing" replication processes and the physical properties of the polymer utilized.

Prof. M. Puska
Helsinki University of Technology, Finland
03-10-2005 through 31-03-2006
Lifetimes of electron-hole excitations at nanostructures on solid surfaces.

Short Visits

Prof. J. Alonso
Universidad de Valladolid, Spain
23-12-2004 through 07-01-2005
Computational simulation of the intercalation of alkaline atoms in graphite and carbon nanotubes. Laser induced fragmentation of atomic clusters.

Prof. I. Nagy
Technical University of Budapest, Hungary
04-01 through 03-02-2005
Various aspects of correlations in extended fermionic systems; spice-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Prof. A. Postnikov
Universität Osnabrück, Germany
25-01 through 06-02-2005
Studies of magnetism in intermetallic compounds, diluted and disordered alloys, and in small clusters/nanoparticles.

Prof. J.A. Sánchez-Gil
Instituto de Estructura de la Materia, CSIC, Spain
25-01 through 26-01-2005
Surface plasmon photonics on surfaces with sub-wavelength structures: from nano-optics on metals to THz waves on semiconductors.

Dr. R. Jansen
University of Twente, Enschede, The Netherlands
27-01 through 30-01-2005
Spin-transport in semiconductor/ferromagnet hybrid structures.

Dr. M. Dubois
IEMN/ISEN/Physique, France
02-02 through 23-02-2005
Scanning tunneling spectroscopy of organic molecules supported on semiconductor and semimetal surfaces.

Dr. V. Tugushev
Russian Research Center "Kurchatov Institute", Moscow, Russia
08-02 through 05-03-2005
Magnetism in superlattices and spintronics.

Dr. A.F. Ho
University of Birmingham, UK
14-02 through 28-02-2005
Effects of disorder in one-dimensional quantum liquids, and phase diagram of binary mixtures of one-dimensional harmonic fluids.

Prof. T. Nagao
Tohoku University, Japan
21-02 through 26-02-2005
Surface phonons and adlayer crystal structures.

Dr. S. Roche
CEA-DSM/DRFMC/SPSMS, France
22-02 through 24-02-2005
Unconventional mesoscopic transport in carbon nanotubes based materials.

Dr. J.O. Fjaerestad
University of Queensland, Australia
24-02 through 01-03-2005
Phase diagram of ladder compounds.

Prof. W. Jaskólski
Institute of Physics Nicholas Copernicus University, Poland
09-03 through 13-03-2005
On peculiar properties of carbon nanotubes.

Prof. J. Alonso
Universidad de Valladolid, Spain
24-03 through 03-04-2005
Computational simulation of the intercalation of alkaline atoms in graphite and carbon nanotubes. Laser induced fragmentation of atomic clusters.

Prof. C. Laubschat
Institut für Festkörperphysik, Germany
31-03 through 01-04-2005
Correlated electronic structure of rare earth systems.

Dr. N. Lorente
Université Paul Sabatier, Toulouse, France
04-04 through 29-04-2005
Metallic and semimetallic nanometer-wide silicon nanowires.

Prof. N. March
Universiteit Antwerpen, Belgium
10-04 through 08-05-2005
Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

Dr. M.S. Gravielle
Instituto de Astronomía y Física del Espacio, Buenos Aires, Argentina
11-04 through 20-04-2005
Atomic collisions and collisions with solids.

Prof. F. Auzel
UMR Groupe d'Optique des Terres Rares, France
12-04 through 28-05-2005
Powder coherent sources both of the superradiant (SR) and Amplified Spontaneous Emission (ASE) types [1,2,3,4].

Doctorand S. Monturet
Université Paul Sabatier, Toulouse, France
18-04 through 20-04-2005
Molecules on surfaces.

Prof. J.M. Alonso Pruneda
ICMAB-CSIC, Barcelona, Spain
24-04 through 29-04-2005
Stopping of slow ions in insulators.

Dr. H. Schwarz
Technische Universität Berlin, Germany
25-04-2005
Gas-phase catalysis by atomic cluster metal ions; the ultimate single-site catalysts.

Dr. J.I. Pascual Chico
Freie Universität Berlin, Germany
27-04 through 29-04-2005
Scanning tunneling spectroscopy.

Prof. G. Morata
Universidad Autónoma de Madrid, Spain
29-04 through 03-05-2005
The three revolutions in biology.

Dr. E. Mena-Osteritz
Universität Ulm, Germany
03-05 through 04-05-2005
Self assembled monolayers.

Prof. J. Pendry
Imperial College, London, UK
15-05 through 20-05-2005
The perfect lens-focusing beyond the diffraction limit.

Prof. J. Inglesfield
University of Wales, Cardiff, UK
15-05 through 19-05-2005
Embedding in photonics and plasmon bands in metallic nanostructures.

Dr. F. Jonsson
EPSRC NanoPhotonics Portfolio Centre, UK
16-05 through 18-05-2005
All optical switching using nano-structural phas transformation.

Prof. H. Petek
University of Pittsburgh, Pennsylvania, USA
23-05-2005 through 26-05-2005
Electron dynamics in time domain.

Prof. B. Hellsing
Chalmers and Göteborg University, Sweden
23-05 through 27-05-2005
Electron-phonon interactions on metal surfaces.

Dr. C. Ambrosch-Draxl
University of Graz, Austria
30-05 through 03-06-2005
Electron dynamics in transition metals.

Prof. A. Galindo
Universidad Complutense de Madrid, Spain
30-05 through 01-06-2005
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. I. Nagy
Technical University of Budapest, Hungary
01-06 through 30-06-2005
Various aspects of correlations in extended fermionic systems; spice-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Prof. V.H. Ponce
Centro Atómico Bariloche, Argentina
30-06-2005
Electron emission in the interaction of light ions with surfaces.

Dr. A. Borissov
Université Paris Sud, France
01-06 through 30-06-2005
Time-dependent density functional theory and wave packet propagation methods.

Dr. G. Bihlmayer
IFF-FZ, Forschungszentrum Jülich, Germany
04-06 through 30-06-2005
Magnetism in low dimensions: Overlayers, wires and atoms.

Prof. U. Heinzmann
Universität Bielefeld, Germany
09-06 through 13-06-2005
Time resolved photoemission.

Dr. J. García de Abajo
Unidad de Física de Materiales, CSIC, Spain
09-06-2005
Simulation of optical properties of complex structures including porous metals and non-spherical nanoparticles. Study of the response of nanostructures and its interactiions with fast electron. Simulation of electron-energy loss spectroscopy cathodoluminescence, and Cherenkov radiation in complex systems.

Prof. N.W. Aschroft
Cornell University, New York, USA
19-06 through 02-07-2005
Theory of many particle systems, density functional, theory (classical and quantum), and theory of dense hydrogen and matter under extreme conditions.

Dr. C. Vallés Callizo
Instituto de Carboquímica, CSIC, Zaragoza, Spain
27-06 through 01-07-2005
Synthesis of carbon nanotubes.

Dr. P.J. Ordejón Rontome
CSIC-ICMB, Barcelona, Spain
01-07 through 30-07-2005
First principles calculations of ballistic transport in nanoscale systems.

Dr. J. Ferrer Rodríguez
Universidad de Oviedo, Spain
06-07 through 08-07-2005
Spin-orbit interaction within the SIESTA method.

Dr. V.M. García Suarez
Universidad de Oviedo, Spain
06-07 through 08-07-2005
Spin-orbit interaction within the SIESTA method.

Dr. G. Bryant
National Institute of Standards and Technology, Gaithersburg, Maryland, USA
21-07 through 23-07-2005
Optoelectronic properties of quantum dots and quantum wires.

Dr. D. Vaknin
Iowa State University, USA
04-08 through 08-08-2005
The magneto-electric effect — a neutron scattering perspective.

Dr. I. Campillo
Euskal Herriko Unibertsitatea/ Universidad del País Vasco, Spain
26-08 through 28-08-2005
Nanostructure of cement-based materials.

Prof. A. Galindo
Universidad Complutense de Madrid, Spain
28-08 through 11-09-2005
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. A.J. da Silva
Universidade de Sao Paulo, Brazil
29-08 through 31-08-2005
Understanding of nanostructures in metals and semiconductors, including metallic nanocontacts, carbon nanotubes, silicon wires, and their interactions with impurities and oxidation.

Doctorand S. Capponi
University of Perugia, Italy
31-08 through 03-09-2005
Dynamics of DNA and proteins by neutron scattering.

Prof. A. Howie
Cavendish Laboratory, Cambridge, UK
01-09 through 15-09-2005
Theory of valence electron excitations by fast electrons.

Dr. F. Schiller
Universität Dresden, Germany
01-09 through 30-09-2005
Crystalline and electronic structure of thin Be and Mg films.

Prof. I. Nagy
Technical University of Budapest, Hungary
02-09 through 29-09-2005
Various aspects of correlations in extended fermionic systems; spice-fluctuation, pair-correlation, one-particle damping, impurity-screening.

Dr. F. Busnengo
Universidad de Rosario, Argentina
08-09 through 07-10-2005
Dissociation of diatomic molecules at surfaces.

Prof. L. Kuipers
Institute for Atomic and Molecular Physics, The Netherlands
12-09 through 13-09-2005
A local(ized) view of nanoscale light propagation.

Prof. B. Braida
Université Pierre et Matie Curie (Paris 6), France
12-09 through 16-09-2005
Theoretical study of SrFe03-x oxygen-vacancy perovskites: GGA versus GGA+U results.

Prof. C. Fadley
Lawrence Berkeley National Laboratory, Californnia, USA
13-09 through 17-09-2005
Some new directions in synchrotron radiation studies of magnetic materials and magnetic nanostructures.

Prof. E. Zaremba
Queens University, Ontario, Canada
15-09 through 30-09-2005
Bose-Einstein Condensation.

Prof. A. Griffin
University of Toronto, Canada
15-09 through 25-09-2005
Ultracold trapped Fermi gases.

Prof. D. Richter
IFF-FZ, Forschungszentrum Jülich, Germany
01-10 through 09-10-2005
Polymer dynamics by neutron techniques.

Prof. A. Salin
Université de Bordeaux I, France
03-10 through 28-10-2005
Dissociation dynamics of diatronic molecules at metal surfaces.

Doctorand T. Hakala
Helsinki University of Technology, Finland
05-10 through 28-10-2005
Lifetimes of electron-hole excitations at nanostructures on solid surfaces.

Prof. J.P. Gauyacq
Université Paris-Sud, France
16-10 through 28-10-2005
Dynamics of excited electrons at adatoms on metal surfaces.

Dr. R. Bergman
Chalmers University of Technology, Göteborg, Sweden
26-10 through 31-10-2005
Systematic studies of the excess wing of glass-formers.

Prof. A. Fernandez Rañada
Universidad Complutense Madrid, Spain
26-10 through 27-10-2005
The Pioneer anomaly as a problem of time dynamics.

Prof. M. Roesler
Hahn-Meitner Institute Berlin, Germany
01-11 through 30-11-2005
Electron emission induced by atomic particles interacting with solids and surfaces.

Dr. G. Darling
University of Liverpool, UK
05-11 through 10-11-2005
Energy exchange between small molecules and metal surfaces.

Dr. K. Starke
Freie Universität Berlin, Germany
09-11 through 11-11-2005
Spectroscopy of magnetic materials.

Prof. P. López Sancho
Instituto de Ciencia de Materiales de Madrid (CSIC), Spain
17-11 through 18-11-2005
New electronic effects in carbon-based materials.

Dr. J. García de Abajo
Unidad de Física de Materiales, CSIC, Spain
22-11 through 23-11-2005
Study of the optical properties of nanostructures using electron microscopy.

Dr. R. Lund
IFF-FZ, Forschungszentrum Jülich, Germany
23-11 through 25-11-2005
Logarithmic chain exchange kinetics of polymeric micelles.

Prof. C. Balbas Ruesgas
Universidad de Valladolid, Spain
24-11 through 25-11-2005
Theoretical study of O2 and CO adsorption on gas phase and supported glod clusters.

Dr. P. Johansson
University of Örebro, Sweden
27-11 through 04-12-2005
Research on the electromagnetic and quantum mechanical response of molecules and nanoparticles in different configurations of experimental interest (STM, Raman, ...).

Dr. J. Bartos
Polymer Institute of SAS, Bratislava, Slovak Republic
28-11 through 06-12-2005
PALS and polymer dynamics.

Prof. A. Seitsonen
Université Pierre et Marie Curie (Paris 6), France
30-11 through 03-12-2005
Density functional theory studies of self-organised organic overlayers on metal surfaces.

Dr. J.M. Alameda Maestro
Universidad de Oviedo, Spain
01-12 through 02-12-2005
Peculiar properties of the magnetization process in magnetic multilayers.

Prof. M. Raizen
University of Texas at Austin, USA
19-12 through 21-12-2005
Ultracold atomic gases.

THE SEMINARS

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2004/05

Y. Moreno Vega
D. Farias Tejerina
I. Egusquiza
M. Verstraete
M.A. Cazalilla
G. Gómez Santos
A. Modinos
C. Díaz Blanco
J.J. Sáenz Gutierrez
X. Obradors
C. Rillo
A. Galindo
E. Ogando
W.A. Hofer
J. Pendry
P. Hofmann
B.S. Mun
H. Koh
F. Flores Sintas
J.D. Fuhr
S. Eremev
R. Hillenbrand
C. Crespos
G.W. Bryant
S. Shabanov
M. Käll
U. Höfer
A. Howie
N. Yamamoto
E. Artacho
M. Trioni
M. Puska
V.N. Strocov
L. Lechuga
S. Molodtsov
N. Lorente
A. Planes
J. Baumberg
D. Vyalikh
T. Teperik

2004/05

J.A. Sánchez-Gil
R. Jansen
A. Postnikov
S. Roche
J.O. Fjaerestad
M.A. Cazalilla
B. Gumhalter
W. Jaskólski
C. Laubschat
M. Silvia Gravielle
H. Schwarz
A.C. Genix
J.I. Pascual Chico
E. Mena-Osteritz
J. Pendry
H. Petek
C. Ambrosch-Draxl
J. García de Abajo
U. Heinzmann
G. Bihlmayer
M.J. Cabrera San Félix
C. Vallés Callizo
N.W. Aschroft
D. Vaknin
A.J. da Silva
S. Capponi
L. Kuipers
C. Fadley
A.Griffin
E. Zaremba
J. P. Gauyacq
A. Fernandez Rañada
R. Bergman
M. Puska
G. Darling
K. Starke
P. Lazic
R. Quirk
P. López Sancho
R. Lund
C. Balbas Ruesgas
A. Seitsonen
J. Bartos

JANUARY 15, 2004
Complex networks in nature: structure and application
Y. Moreno Vega (Universidad de Zaragoza, Spain)

JANUARY 16, 2004
Phonon softening, chaotic motion and order-disorder transition in Sn/Ge(111)
D. Farias Tejerina (Universidad Autónoma de Madrid, Spain)

JANUARY 23, 2004
Time in quantum mechanics
I. Egusquiza (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)

JANUARY 29, 2004
Interactions between carbon and transition metal elements
M. Verstraete (PCPM, Louvain-la-Neuve, Belgium)

JANUARY 30, 2004
News and promises from NanoKelvinLand: Strongly correlated ultracold atoms
M.A. Cazalilla (ICTP Trieste, Italy)

FEBRUARY 6, 2004
Wave propagation in left-handed systems
G. Gómez Santos (Universidad Autónoma de Madrid, Spain)

FEBRUARY 11, 2004
Photonic and phononic crystals
A. Modinos (National Technical University of Athens, Greece)

FEBRUARY 20, 2004
Can we study H2/Pd(111) interactions using classical dynamics?
C. Díaz Blanco (Universidad Autónoma de Madrid, Spain)

FEBRUARY 24, 2004
Light-induced resonant forces between particles in a waveguide
J.J. Sáenz Gutiérrez (Universidad Autónoma de Madrid, Spain)

MARCH 4, 2004
Superconductividad: Nuevos retos para el siglo XXI
X. Obradors (ICMB-CSIC, Spain)

MARCH 26, 2004
Electrical quantum metrology
C. Rillo (CSIC-Universidad de Zaragoza, Spain)

MAY 6, 2004
Quantum information with applications to teleportation, cryptography and computation
A. Galindo (Universidad Complutense de Madrid, Spain)

MAY 7, 2004
Quantum size effects in Pb thin films on Cu(111): Electronic-structure calculations
E. Ogando (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)

MAY 11, 2004
Quantum information with applications to teleportation, cryptography and computation
A. Galindo (Universidad Complutense de Madrid, Spain)

MAY 12, 2004
Towards real-time high-resolution STM analysis: Eyes for technology on the nanoscale
W.A. Hofer (University of Liverpool, UK)

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Quantum information with applications to teleportation, cryptography and computation
A. Galindo (Universidad Complutense de Madrid, Spain)

MAY 14, 2004
Recent results on materials with negative refraction index
J. Pendry (Imperial College, London, UK)

MAY 19, 2004
Some unresolved problems in electron spectroscopy from graphite
P. Hofmann (University of Aarhus, Denmark)

MAY 20, 2004
A study of the electronic structure of Pd thin films on Re(0001) and Pt(111) by high-resolution core level and valence band photoemission
B.S. Mun (Lawrence Berkeley National Laboratory, California, USA)

MAY 20, 2004
Angle-resolved photoemission spectroscopy and its application to ultra-thin In and Pb overlayers on Si(111)
H. Koh (Lawrence Berkeley National Laboratory, California, USA)

MAY 20, 2004
Quantum information with applications to teleportation, cryptography and computation
A. Galindo (Universidad Complutense de Madrid, Spain)

MAY 21, 2004
Nanowires: from breakjunction contacts to step-edge decorated lines
F. Flores Sintas (Universidad Autónoma de Madrid, Spain)

MAY 25, 2004
Quantum information with applications to teleportation, cryptography and computation
A. Galindo (Universidad Complutense de Madrid, Spain)

JUNE 1, 2004
Quantum information with applications to teleportation, cryptography and computation
A. Galindo (Universidad Complutense de Madrid, Spain)

JUNE 11, 2004
Electronic structure of point defects on the MoS2(0001) surface
J.D. Fuhr (CRMCN-CNRS, Marseille, France)

JUNE 14, 2004
Phonons in alcali metals adlayers on aluminium surfaces
S. Eremev (Institute of Strength Physics and Materials Sciences, Tomsk, Russia)

JUNE 17, 2004
Scattering-type near-field microscopy for optical /infrared nanoanalytics
R. Hillenbrand (Max-Planck Institut, Martinsried, Germany)

JUNE 28, 2004
Dynamics of gas-surface reactions: theoretical study of H_2 dissociation on Pd(111) surface
C. Crespos (Laboratoire de Physico-Chimie Moleculaire, Bordeaux, France)

JULY 9, 2004
Lighting the nanoworld
G.W. Bryant (National Institute of Standards and Technology, Gaithersburg, USA)

JULY 23, 2004
On pseudospectral methods of solving maxwell's equations for passive media
S. Shabanov (University of Florida, USA)

JULY 30, 2004
Nanoplasmonics and single molecule spectroscopy
M. Käll (Chalmers University of Technology, Gotheborg, Sweden)

SEPTEMBER 6, 2004
Time-resolved two-photon photoemission of Ar/Cu interface states
U. Höfer (Philipps- Universität Marburg, Germany)

SEPTEMBER 15, 2004
Recent progress and further opportunities for spatially localised spectroscopy
A. Howie (Cavendish Laboratory, Cambridge, UK)

SEPTEMBER 7, 2004
Electron beam induced light emission from surface plasmon on metallic photonic crystals
N. Yamamoto (Tokyo Institute of Technology, Japan)

SEPTEMBER 26, 2004
A condensed matter physicist in an earth sciences department
E. Artacho (University of Cambridge, UK)

OCTOBER 27, 2004
Theory of metastable deexcitation spectroscopy on simple metals: Ab initio versus approximate approach
M. Trioni (Università di Milano-Bicocca, Italy)

November 4, 2004
Light-induced resonant forces between particles in a waveguide
J.J. Saenz Gutierrez (Universidad Autónoma de Madrid, Spain)

November 4, 2004
Two-dimensional electron gas in quantum dots under high magnetic fields
M. Puska (Helsinki University of Technology, Finland)

November 9, 2004
Dispersions and lifetimes of photoemission final states by very-low-energy electron diffraction (VLEED) implications for photoemission band mapping in 3D k-space
V.N. Strocov (S.P. Scherrer Institute, Switzerland)

November 9, 2004
Integration of micro/nanotechnologies with nanobiotechnology: fully-operated biosensing platforms
L. Lechuga (Centro Nacional de Microelectrónica (CNM)-CSIC Madrid, Spain)

NOVEMBER 19, 2004
Electronic structure of regular bacterial surface layers
S. Molodtsov (Technische Universität, Dresden, Germany)

NOVEMBER 23, 2004
Metallic and semimetallic nanometer-wide silicon nanowires
N. Lorente (Université Paul Sabatier, France)

NOVEMBER 25, 2004
Extended first-order transitions in solids: A new view
A. Planes (Universidad de Barcelona, Spain)

DECEMBER 2, 2004
Chameleon metals: Photonic nanostructures from self-assembly
J. Baumberg (University of Southampton, UK)

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Quantum Well States in bilayers of Ag and Au metals
D. Vyalikh (Technische Universität Dresden, Germany)

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Void plasmons and total absorption of light on nanoporous surface of metal
T. Teperik (Institute of Radio Engineering and Electronics, Russian Academy of Sciences, Russia)

JANUARY 26, 2005
Surface plasmon photonics on surfaces with sub-wavelength structures: From nano-optics on metals to THz waves on semiconductors
J.A. Sánchez-Gil (Instituto de Estructura de la Materia, CSIC, Spain)

JANUARY 28, 2005
Spin-transport in semiconductor/ferromagnet hybrid structures
R. Jansen (University of Twente, Enschede, The Netherlands)

JANUARY 31, 2005
Magnetic interactions in molecular magnets
A. Postnikov (Universitaet Osnabrueck, Germany)

FEBRUARY 23, 2005
Unconventional mesoscopic transport in carbon nanotubes based materials
S. Roche (CEA-DSM/DRFMC/SPSMS, France)

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Orbital currents and d-density waves in strongly correlated electron systems
J.O. Fjaerestad (University of Queensland, Australia)

MARCH 7, 2005
Quasi-1D systems: From 'model' solid state materials to quantum engineering with cold fermionic atoms
M.A. Cazalilla (DIPC, Spain)

MARCH 9, 2005
Ultrafast electron dynamics and decoherence in surface bands
B. Gumhalter (University of Zagreb, Croatia)

MARCH 11, 2005
On peculiar properties of carbon nanotubes
W. Jaskólski (Institute of Physics Nicholas Copernicus University, Poland)

APRIL 1, 2005
Correlated electronic structure of rare earth systems
C. Laubschat (Institut für Festkörperphysik, Germany)

APRIL 15, 2005
Interference effects in electron capture from insulator surfaces
M. Silvia Gravielle (Instituto de Astronomía y Física del Espacio, Buenos Aires, Argentina)

APRIL 25, 2005
Gas-phase catalysis by atomic cluster metal ions: The ultimate single-site catalysts
H. Schwarz (Technische Universität Berlin, Germany)

APRIL 28, 2005
The Dynamics of poly (ethylene oxide) in a blend with poly (methyl methacrylate)
A.C. Genix (Thiais Université Paris XII, France)

APRIL 29, 2005
"Visualization" of electronic states at surfaces
J.I. Pascual Chico (Freie Universität Berlin, Germany)

MAY 4, 2005
2D and 3D self-assembly of organic semiconductors
E. Mena-Osteritz (Universität Ulm, Germany)

MAY 14, 2005
Recent results on Materials with Negative Refraction Index
J. Pendry (Imperial College, London, UK)

MAY 25, 2005
Ultrafast imaging of surface plasmons dynamics
H. Petek (University of Pittsburgh, Pennsylvania, USA)

JUNE 1, 2005
Excitonic effects in the absorption spectra of organic semiconductors
C. Ambrosch-Draxl (University of Graz, Austria)

JUNE 9, 2005
Lattice, site, and plasmon resonances in structured metal films
J. García de Abajo (Unidad de Física de Materiales, CSIC, Spain)

JUNE 10, 2005
Phase and attosecond-time resolved photoemission experiments
U. Heinzmann (Universität Bielefeld, Germany)

JUNE 15, 2005
Nanoscale magnetism from first principles
G. Bihlmayer (IFF-FZ, Forschungszentrum Jülich, Germany)

JUNE 17, 2005
Molecular modelling of water ice in atmospheric and astrophysical environments.
M.J. Cabrera San Félix (DIPC, Spain)

JUNE 28, 2005
Synthesis of carbon nanotubes
C. Vallés Callizo (Instituto de Carboquímica, CSIC, Zaragoza, Spain)

JULY 1, 2005
Higher superconductivity in the dense lower elements
N.W. Aschroft (Cornell University, USA)

AUGUST 5, 2005
The magneto-electric effect — a neutron scattering perspective
D. Vaknin (Iowa State University, USA)

AUGUST 30, 2005
Computer simulations of atomically thin gold nanowires and of defects in carbon nanotubes
A.J. da Silva (Universidade de Sao Paulo, Brazil)

AUGUST 31, 2005
DNA dynamics in a glassy matrix as a function of the hydration
S. Capponi (Università degli studi de Perugia, Italy)

SEPTEMBER 13, 2005
A local(ized) view of nanoscale light propagation
L. Kuipers (Institute for Atomic and Molecular Physics (AMOLF), The Netherlands)

SEPTEMBER 14, 2005
Some new directions in synchrotron radiation studies of magnetic materials and magnetic nanostructures
C. Fadley (Lawrence Berkeley National Laboratory, USA)

SEPTEMBER 21, 2005
An overview of recent work on trapped Fermi superfluid gases
A.Griffin (University of Toronto, Canada)

SEPTEMBER 27, 2005
Vortices in trapped Bose gases
E. Zaremba (Queens University, Canada)

OCTOBER 21, 2005
Image states on finite size adsorbate islandes
J. P. Gauyacq (Université Paris Sud, France)

OCTOBER 26, 2005
The Pioneer anomaly as a problem of time dynamics
A. Fernandez Rañada (Universidad Complutense de Madrid, Spain)

OCTOBER 27, 2005
Systematic studies of the dielectric excess wing of glass-formers
R. Bergman (Chalmers University of Technology, Göteborg, Sweden)

NOVEMBER 4, 2005
Finite-element implementation of the non-equilibrium Green's function scheme for electron transport through nanostructures
M. Puska (Helsinki University of Technology, Finland)

NOVEMBER 9, 2005
Energy exchange between small molecules and metal surfaces
G. Darling (University of Liverpool, UK)

NOVEMBER 11, 2005
Rashba effect and spin dynamics in 2-dimensional 4f electron systems
K. Starke (Freie Universität Berlin, Germany)

NOVEMBER 16, 2005
The Robin Hood Method - a new view on differential equations
P. Lazic (Rudker Boskovic Institute, Zagrev, Croatia)

NOVEMBER 17, 2005
Basic concepts of anionic polymerization for physicists
R. Quirk (The University of Akron, Ohio, USA)

NOVEMBER 18, 2005
New electronic effects in carbon-based materials
P. López Sancho (Instituto de Ciencia de Materiales de Madrid (CSIC), Spain)

NOVEMBER 25, 2005
Logarithmic chain exchange kinetics of polymeric micelles
R. Lund (IFF-FZ, Forschungszentrum Jülich, Germany)

NOVEMBER 25, 2005
Theoretical study of O2 and CO adsorption on gas phase and supported glod clusters
C. Balbas Ruesgas (Universidad de Valladolid, Spain)

DECEMBER 1, 2005
Density functional theory studies of self-organised organic overlayers on metal surfaces
A. Seitsonen (Université Pierre et Marie Curie, France)

DECEMBER 2, 2005
Positron annihilation lifetime spectroscopy in glasses and polymers
J. Bartos (Polymer Institute of SAS, Bratislava, Slovak Republic)

DECEMBER 2, 2005
Peculiar properties of the magnetization process in magnetic multilayers
J.M. Alameda Maestro (Universidad de Oviedo, Spain)

DECEMBER 20, 2005
Experiments with a "Particle in a Box": Bose Einstein condensates, and Maxwell's Demon
M. Raizen (University of Texas at Austin, USA)

THE WORKSHOPS

DIPC facilitates the exchange of information and establishment of new creative research collaborations between attending scientists.

2004/05

1st NanoSpain Workshop

MARCH 10-12, 2004

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Prof. J. Veciana (Instituto de Ciencia de Materiales de Barcelona/CSIC, Spain)

During the last two decades, a revolutionary scientific new age, based on the capacity to observe, characterize, manipulate and organize matter in the nanometric scale, is appearing. In this scale, physics, chemistry, materials science, computational theory, and engineering converge towards the same theoretical principles and experimental findings that are basically governed by the laws of Quantum Mechanics. Nanotechnology involves these interdisciplinary knowledge areas and methodologies in order to study, manufacture and characterize functional structures with dimensions of tens of nanometers.

The three year-old NanoSpain network aims to agglutinate and coordinate the efforts made in the field of Nanotechnology by Spanish groups from universities, research institutes and companies. Moreover, this network has tried to help the government institutions in defining potential actions and plans referring to this area. Currently, the NanoSpain network, comprised of 111 Spanish groups with nearly 400 researchers in total, is one of the largest Spanish scientific networks.

As a direct and most effective way to enhance the interaction between network members, the first meeting of NanoSpain has been organised. Its objective is to facilitate the dissemination of knowledge and promote interdisciplinary discussions among the different NanoSpain groups. In order to organise the various sessions and to select contributions, the meeting has been structured in the following thematic lines, but interactions among them will be promoted:

- MEMS/NEMS
- Nanobiology
- Nanomaterials
- Nanochemistry
- Nanoelectronics
- Scanning Probe Microscopies (SPM)
- Scientific Policy and Infrastructure
- Simulation at the nanoscale

Another objective of this meeting was to consider the state of Nanotechnology in Spain, as well as in reaching conclusions concerning the future of the NanoSpain network, in order to guarantee its continuity by means of concrete proposals and a renovation of its structures.

This event receives funding from Donostia International Physics Center (DIPC) and the Spanish Ministry of Science through the following two networks:

- Red Española de Nanotecnología (NANOSPAIN)
  Funding Agency: Ministerio de Ciencia y Tecnología — Acción Especial (MAT2001-5411-E)
- Red Nacional de Investigadores en Nanociencias: Metodologías Experimentales y Teóricas (NANOCIENCIA)
  Funding Agency: Ministerio de Ciencia y Tecnología — Acción Especial (PGC2000-2586-E)

CONTRIBUTIONS

J. Brugger	**Mems-based nanopatterning and nems**
J. Bausells	**Fabrication of micro/nano electromechanical devices in silicon**
J. Gonzalez	**Smco hard magnetic films for mems devices**
C.A. Mills	**Nanopatterning of polymer surfaces for biomedical applications**
M. Aguirregabiria	**Novel 3d embedded microfluidic channels for biomems applications**
S. Yaliraki	**Controlling self-assembled architectures for optimal molecular electronic devices**
M.J. Caturla	**Modeling material behavior at the nanoscale using molecular dynamics: nanocrystals and nanocontacts**
J.I. Cerdá	**An stm study of water on pd(111):experiment and theory**
M. Machado	**Distance dependent standing wave pattern induced by a benzene molecule adsorbed on a cu(111) surface**
J.J. Sáenz	**Electrostatic forces in scanning probe microscopy: quantitative analysis of the electrostatic signal in nanowires**

J. Barth	**Engineering supramolecular nanosystems at surfaces**
J.A Alonso	**Interaction of hydrogen with carbon nanotubes**
D.B. Amabilino	**Self-assembly of components for nanometerscale molecular electronics—tetrathiafulvalene monolayers studied by stm**
M. Clemente-León	**Nanostructured hybrid molecular materials**
J.V. García-Ramos	**Raman and infrared spectroscopy on nanostructured metal surfaces (sers and seir) of extremely dispersed or isolated molecular systems**
M.Victoria Martinez	**Towards metallophthalocyanine-based molecular materials with electronic and optoelectronic properties**
B. Onoa	**Nucleic acids: tools and targets in nanotechnology**
R. Eritja	**Assembly of nanomaterials directed by oligonucleotide derivatives**
I. Katakis	**Site directed immobilisation of biorecognition nanomodules for biochips**
I. Casuso	**Advances towards the development of scanning probe microscopy for the electrical characterisation of biological samples**
M. Vazquez	**National strategic action plan of nanotechnology**
M. Miles	**Developments in spm for nanotechnology**
A.M. Baró	**Characterization by atomic force microscopy of biological material under physiological conditions**
R. García	**Liquid bridges, force microscopy and nanofabrication**
F. Pérez Murano	**Measurement of electrical current during scanning probe oxidation**
H. Suderow	**Advances and future prospects of the use of superconducting tips in very low temperature stm**
Y. Horikoshi	**Mbe for semiconductor nanostructures**
B. Garrido	**Development of microphotonic devices based on nanocrystalline silicon**
J. Fernández-Rossier	**Ferromagnetism in diluted magnetic semiconductor single electron transistor**
T. Gonzalez	**Monte carlo simulation of ballistic nanodevices for thz applications**
J.L. Vicent	**Superconducting reversible nanorectifier based on the ratchet effect**
D. Mecerreyes	**Design of nanomaterials for electrochemical applications**
A. Asenjo	**Arrays of magnetic nanowires in alumina membranes**
D. Ruiz-Molina	**Multiple length scale patterning of single-molecule magnets**

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J. Esquena	**Preparation of mesoporous silica templated in highly concentrated emulsions**
J. Bartolomé	**Anomalous low-temperature behavior of switching fields in fe nanowires**
P. Gomez-Romero	**Hybrid nanocomposite materials for energy storage and conversion applications**
R. Miranda	**Magic heights in pb nanodots induced by quantum size effects**
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P. Van-Hove	**Advanced research in nanotechnology information devices and nanoelectronics: contribution of ec programmes**
C. Domínguez	**Facilities expansion for nanoand micro fabrication at the imb-cnm.**
E. Prieto	**The metrological infrastructure and the "nano" world**
J. Samitier	**Nanotechnology platform at Barcelona science parknanophotonic**
M.A. Cazalilla	**Strongly correlated atoms in two-dimensional optical lattices**
J.J. Sáenz	**Photonic liquids**
L.A. Blanco	**Control of spontaneous emission by means of nanostructures**
B. Garrido	**Electroluminescence, optical memories, and optical amplification from nanostructured group iv semiconductors: towards integration of photonic devices with si technology**

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III Reunión Nacional de Física del Estado Sólido

JUNE 2-4, 2004

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Following the tradition of the two previous meetings (Madrid, 2000 and Calella, Barcelona, 2002) the third national conference of the Condensed Matter Group ("Grupo Especializado de Física del Estado Sólido", GEFES) of the Spanish Royal Physical Society was organized in San Sebastian in June 2004. The general aim of these series of meetings is to put together Spanish people working in the different areas of condensed matter physics and related topics. On the other hand, these meetings try to offer young researchers the opportunity of presenting their work in a frank atmosphere and to have plenty of time for discussions with senior and established scientists

CONTRIBUTIONS

D. Richter	**Neutrons in Soft Matter Science**
J. Fernández Rossier	**Control eléctrico de nano-imanes semiconductores**
A. Masquaraque	**Ondas de densidad de carga en sistemas de baja dimensionalidad**
A. Palau	**Corriente percolativa y anclaje de vórtices en cintas superconductoras de $Yba_2Cu_3O_7$**
F. Pérez Murano	**Fabrication of mechanical devices**
S. Arrese-Igor	**Estudio de la dinámica de los anillos fenileno de la polisulfona vítrea mediante dispersión de neutrones: escalas micro y mesoscópica**
A. Hdez. Vozmediano	**Local defects and ferromagnetism in graphite**
F. Rivadulla	**Segregación de fases en manganitas: ¿un sistema de partículas interaccionantes?**
F. Meseguer	**Colloidal crystals as photonic crystals**
T. Ezquerra	**Fenómenos de ordenamiento en sistemas poliméricos investigados mediante técnicas de relajación dieléctrica**
L.M. Liz Marzán	**Nanocilindros metálicos, formación, propiedades ópticas y estructuración**
O. Fesenko	**Simulation of switching properties of Fe Pt/Fe Rh films for heat-assisted magnetic recording application**
I. Fernández Barquín	**Interacciones indirectas y dipolares en aleaciones nanométricas de Fe-Cu-Ag**
M. Salmerón	**The structure of surfaces in thermodynamic equilibrium with high pressure environments**
A. Bergara	**Aleaciones metálicas de hidrógeno, ¿posibles superconductores de alta temperatura?**
J. Villegas	**Superconductores nanoestructurados artificialmente: la dinámica de vórtices bajo control**
J. Stankiewicz	**Interrelación entre transporte electrónico y magnetismo en aleaciones intermetálicas**
A. Asenjo	**Microscopía de fuerzas magnéticas**
M.D. Martín	**Hacia la condensación de polaritones en microcavidades de semiconductor**
J. Gil Sevillano	**Efectos de tamaño en plasticidad cristalina Mesa Redonda: "Trends and Interdisciplinariety in condensed matter physics" moderado por P.M. Echenique, con la participación de M. Salmerón, J. Tejada y M. Vázquez.**
J. García	**Radiación de sincrotrón: Dispersión Resonante de Rayos X.**
J.L. García Muñoz	**Separación de fases y localización electrónica en óxidos: complementariedad de la difracción sincrotrón y de neutrones.**
C. Tejedor	**Usando puntos cuánticos para hacer óptica cuántica**
A. Baró	**Microscopías de proximidad y microscopía electrónica**
B. Martínez	**Ferromagnetism in wide bandgap semiconductors: Co-doped ZnO particles**
D. Ruiz Molina	**Multiple length scale patterning of single molecule magnets**
A. Arnau	**Forma atómica e inversión de contraste en imágenes STM**
J.G. Rodrigo	**Estudio de la superconductividad multibanda en NbSe2 mediante STM con punta superconductora**
M.J. Caturla	**Modelización de materiales irradiados y nanoestruturas**
A. Postigo	**Fabrication and characterization of 2D photonic crystals in GaInAsP/InP semiconductor laser heterostructures**

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International Workshop: Photonic and Electronic Materials

JUNE 14-16, 2004

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

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

CONTRIBUTIONS

P. N. Prasad	**Emerging opportunities in Nanophotonics and Biophotonics**
P. Fleitz	**Understanding the photophysics of two-photon absorbing materials**
J. Ripoll	**Non contact optical tomography for 3D imaging in tissue**
P. Günter	**DAST crystals and thin films for electro-optics and THz generation**
T. Kaino	**Fabrication of polymer optical waveguides using soft-lithography**
D.R. Evans	**Understanding and eliminating photovoltaic induced instabilities during contra-directional two-beam coupling in photorefractive LiNbO3:Fe**
I. Ledoux	**Multifunctional molecular materials and nanostructures for optical signal processing**
D. Levy	**Electrooptical properties of gel-glass dispersed liquid crystals (GDLCs) devicesby chemical modification of hybrid silica/liquid crystal interfaces**
J. L. Serrano	**Supramolecular organizations based on liquid crystals for molecular electronic applications**
J. Martorell	**Counter-propagating nonlinear interaction in photonic structures**
V. M. Orera	**Novel photonic materials made from ionic eutectic compounds**
F. J. García de Abajo	**Multiscale metamaterials**
S. John	**Photonic band gap materials: Semiconductors of light**
F. Meseguer	**Sonic crystals and new phenomena in periodic systems**
C. López	**Materials aspects of opals as photonic crystals for devices**
W.M. Yen	**General factors governing the efficiency of luminescence devices**
G. Boulon	**Optical spectroscopy, concentration quenching mechanisms and theoretical approach of laser performances in Yb3+-doped oxide garnets**
H. U. Güdel	**New upconversion light emitting materials**
K. Ueda	**Ceramics lasers, today and future**
B. Di Bartolo	**Upconversion dynamics in Pr-doped YAG and YAlO3 laser crystals**
F. Auzel	**Powder Lasers: Stimulated amplification versus super-radiance**
N.P. Barnes	**Compositionally tuned lasers practical lasers at designer wavelengths**
D. Vivien	**Ytterbium activated materials: New opportunities for solid-state lasers**

R.M. Almeida	**Novel glassy and nanocrystalline photonic materials**
G.C. Righini	**Integrated optical amplifiers and microspherical lasers based on erbium-doped oxide glasses**
J.-L. Adam	**Non-oxide photonic glasses and waveguides**
L. Viña	**Non-linear effects in the ultrafast emission from semiconductor microcavities**
G.M. Turner	**Small animal imaging with fluorescence tomography**

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Molecule Surface Interactions: Elementary Reactive Processes

SEPTEMBER 7-11, 2004

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Reactivity at gas-solid interfaces plays a fundamental role in a large number of natural processes: heterogenous catalysis, atmospheric reactions, interstellar matter, biological or geological media. Recently, reactivity studies have greatly benefited from the development of individual atom, molecule or radical manipulation and reaction control on surfaces. The latter technique allows to pilot step by step chemical reactions, to observe elementary reactions in real time, to construct nanostructured catalysts, etc. Molecular beams allow to simulate elementary steps in catalytic processes like the formation and stabilization of reactive radicals or direct reactions between adsorbates and atoms/molecules of the gas phase. On the other hand, theoretical methods for the determination of the electronic structure of adsorbates on surfaces have reached the point where they are able to deal with complex situations, like the determination of reactive paths, even when the latter involve defects or local modifications of the surface. The concerted theoretical and experimental approach has proven to be very successful for the elucidation of elementary microscopic reaction steps of molecules at surfaces. In this workshop, the current state of the art in both theory and experiment was reviewed and promising new developments discussed.

CONTRIBUTIONS

A. Kleyn	**Reactive processes at the surfaces of a fusion reactor**
R. Beck	**State resolved studies of molecule- Surface reaction dynamics**
G. Sitz	**State resolved studies of the scattering of D2 and HD from Pd(111)**
M. Rocca	**Stereodynamics of hydrocarbon adsorption at Ag surfaces**
K.H. Rieder	**STM control of chemical reactions**
N. Lorente	**Inducing controlled atomic dynamics by an electron current**
H. Ueba	**Theory of inelastic tunneling and its relation to vibrational excitation in ladder climbing process of single adsorbates**
C. Corriol	**Role of surface geometry and electronic structure in STM images of O/Ru(0001) surfaces**
F. Zaera	**Selectivity in catalysis explained by the mechanisms of surface reactions**
L. Savio	**Adsorption dynamics of simple molecules at surfaces with well defined defects: O2 and C2H4/Ag(n10)**
B. Hayden	**Dissociation dynamics on stepped metal surfaces**
R. Olsen	**Why rough surfaces make good catalysts?**
A. Dianat	**Hydrogen dissociation dynamics on transition metal surfaces**
W. Dong	**Trapping, molecular adsorption and precursors for nonactivated chemisorption**
U. Hoefer	**Angular and vibrational dependent dynamics of hydrogen adsorption on Si (001)**
A. Luntz	**How adiabatic is activated adsorption?**
H. Nienhaus	**Electronic excitations by reactive particle-surface interaction**
M. Persson	**Electronically, non-adiabatic processes in molecule-surface interactions**
K. Reuter	**The steady-state of heterogeneous catalysis, studied by first principles statistical mechanics**
A.C. Kummel	**Anisotropic angular distributions of ejected Cl atoms from the abstractive chemisorption of Cl2 on Al(111)**
J. Manson	**Scattering of molecules by surfaces**
F. Martín	**Reflection and dissociation of H2 and D2 molecules on Pd and NiAl surfaces**

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Polymer-based Complex Systems Workshop

JANUARY 24-25, 2005

Organizers
Donostia International Physics Center, Spain
Forschungszentrum Jülich, Germany
Prof. J. Colmenero (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)

The SoftComp Area 4 meeting "Polymer-based complex systems workshop" was the first of the periodic meetings of the SoftComp network focused on the topic covered by this area.

CONTRIBUTIONS

J. Colmenero
Welcome and General information about SoftComp

W. J. Briels
Coarse Graining of Polymer Melts

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Molecular Stretching in Polymer Melts undergoing steady elongational flow

W. Pyckhout-Hintzen
An interplay of SANS and Rheological Relaxation Data in Deformed Melts

J. Claracq
Tailoring Polymer Topology for Improved Melt Strength

A. Alegría
Segmental Dynamics in Polymer Blends by Broad Band Dielectric Spectroscopy

J. Colmenero
Segmental Dynamics in Polymer Blends by Quasielastic Neutron Scattering

A. Wischnewski and M. Zamponi
Microscopic dynamics in Polymer Systems investigated by Neutron Spin Echo Spectroscopy

A. Likhtman
Search for the Fundamental Model of Entanglements

N. Inkson
Structural Architecture of Branched Polymers and Processing Modeling

P. J. Hine
Understanding the links between structure and properties in 2 phase polymer composites

T. C. B. McLeish
Predictive Rheology of Highly-Branched Polymer Ensembles

D. Vlassopoulos
Studies of the dynamics of complex polymer systems

R. Tuinier
Phase behaviour of dispersions of spheres and stiff chains

R. Zorn
Confinement Effects on the Dynamics of Glass Forming Liquids and Polymers

W. Paul
A Nanobuoy Floating on a Polymer Film

I. Pastoriza-Santos
Nanoparticle-Doped Polydimethylsiloxane Elastomer Films

L. M. Liz-Marzán
Optical Control and Patterning of Gold Nanorod-PVA Nanocomposites Films

J. Oberdisse
Structure of silica aggregates in a soft polymeric matrix by SANS

J. Colmenero
General Information and Discussion: SoftComp MoU and SoftComp Applications

Current Status of Activities: Workpackage 4.1 (Tailoring Rheological and mechanical Properties: A molecular Approach)

Current Status of Activities: Workpackage 4.2 (Reinforcement by Internal Surfaces in Polymer Nanofiller Composites)

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Dynamics of Polymer Blends Workshop

JUNE 2-4, 2005

Organizers
Donostia International Physics Center, Spain
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The focus of this workshop was the critical revision of the state of the art and future perspectives regarding the question of the dynamic miscibility in polymer blends. This can be formulated as: How does blending affect the different dynamical processes taking place in a polymer? Especially interesting is the influence on the structural relaxation, process directly related to the phenomenon of the glass transition. Intense scientific activity has been developed during the last two decades to solve this problem from both, theoretical and experimental viewpoints. General consensus on the well established phenomenological observations as well as on the successes and failures of the current theoretical approaches was achieved by the participants, who can be considered as the most recognized scientists currently dealing with this subject worldwide.

CONTRIBUTIONS

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Dynamics in Miscible Blends: Recent Results and Open Questions

D. Richter
Dynamic Miscibility in Polymer Blends—A Quasielastic Neutron Scattering Approach

C. Lorthoir
Local dynamics in miscible poly(styrene)-poly(vinyl methyl ether) blends below the glass transition temperature: Out of equilibrium dynamics of poly(vinyl methyl ether) segments

J.K. Maranas
An atypical case of blend dynamics: the PEO/PMMA blend

A. Arbe
Quasielastic Neutron Scattering Study on the Effect of Blending on the Dynamics of Head-to-Head Poly(propylene) and Poly(ethylene propylene)

S.K. Kumar
Importance of Concentration Fluctuations in the Dynamics of Miscible Polymer Blends

D. Canghialosi
Thermodynamic approach to describe the component dynamics in miscible polymer blends

K. Adachi
Dielectric Study of Dynamical Hetrogeneity in Blends of Polyethers and Interpretation with a Gear Model

M. Ediger
Segmental and Terminal Dynamics in Miscible Blends Containing Polyisoprene or Polystyrene.

J. Haley
Dynamics in miscible polymer blends: the relationship—or lack thereof—between global and local motions

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A Description of the Dynamics in Miscible Blends based on the Coupling Model

G. Fytas
Rich Dynamics in Diblock Copolymers

G. Floudas
Effects of pressure on blend dynamics

E. Leroy
Modelling the dynamics of polymer blends: Direct and inverse problems, and the importance of experimental Tg measurements

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Summer School on Metamaterials for Microwaves And Optical Technologies

JULY 18-20, 2005

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Metamaterials constitute artificial media that are structured in order to sustain electromagnetic properties that are not available in nature. This summer school intends to provide the attendents with a global understanding of the state-of-the-art of this area of research. This goal will be realized by means of invited talks given by internationally renown researchers, as well as by active participation of young researchers, who will have the opportunity to present their achievements within activities specifically targeted for them. Furthermore, we intend to stimulate the relationship between basic research and industry that such excellent results is producing in telecommunications and information technologies.

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V.G. Veselago	**Some remarks to electrodynamics of materials with negative refraction**
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V.M. Shalaev	**Optical negative index materials**
N. Yamamoto	**Light emission by surface plasmon on metal nanostructures induced by high energy electrons**
A.G. Schuchinsky	**Surface plasmons in layered semiconductor dielectric structures**
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J.C. Vardaxoglou	**Metallodielectric EBG Surfaces: Miniaturisation, tenability and antenna applications**
P. de Maagt	**Electromagnetic bandgap antennas and components for microwave and submillimetre wave applications**
M. Sorolla	**Antennas based upon enhanced microwave transmission**
T. Taubner	**Nanomechanical resonance tuning in optical near field interaction**
A.K. Iyer	**Negative-refractive-index transmission-line metamaterials and applications**
B. Jecko	**Overview of the EBG Resonator Antenna**
S. John	**Photonic band gap materials: Engineering the fundamental properties of light**
C. López	**Wealth of materials and functionalities for composite opals**
K. Guven	**Development and analysis of metamaterials with negative index of refraction**
G.W. Bryant	**The nanooptics of coupled metallic nanoparticles**
P. Johansson	**Quantum optics treatment of surface-enhanced raman scattering and fluorescence**
J. Pérez Juste	**Gold nanorods: Properties and structuration**
C.M. Soukoulis	**Negative index materials: New frontiers in optics**
L. Martín Moreno	**Wave transmission through apertures assisted by surface states**
A. Rubio	**Optical properties of nanostructures and biomolecules from first principles**
J.J. Sáenz	**Unusually strong optical interactions between particles in a waveguide**

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Workshop in Honor of Antoine Salin:

Recent Advances on the Dynamics of Atomic and Molecular Particles Interacting With Gas and Solid Targets

OCTOBER 24-25, 2005

Organizers
Prof. A. Arnau (Universidad del Pais Vasco/Euskal Herriko Unibertsitatea, Spain)
Dr. H.F. Busnengo (Universidad de Rosario, Buenos Aires)
Dr. C. Crespos (Universite de Bordeaux, France)
Dr. R. Diez Muino (Unidad de Fisica de Materiales, CSIC, Spain)
Prof. P.M. Echenique (Donostia International Physics Center and
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)

As an expression of respect and gratitude to the scientific career of Antoine Salin, and due to his recent retirement, a scientific workshop was held in Donostia - San Sebastian at the end of October. The workshop included several sessions on different hot topics of active research in the fields of gas-surface dynamics, atomic collisions in the gas and solid phases, and other related subjects.

CONTRIBUTIONS

ION-SOLID INTERACTIONS

P. Bauer **Electronic stopping of slow hydrogen Ions in metals and insulators**

J.E. Miraglia **Plasmon decay mechanisms in proton metal collisions**

V. H. Ponce **Convoy electrons: from ion-atom to ion-surface collisions**

G. Schiwietz **Auger spectroscopy for short-time ion-solid interactions**

J. García de Abajo **Electron energy loss as a probe of photonic structures**

ATOMIC AND MOLECULAR PHYSICS

P.N. Abufager **Single electron capture involving multielectron atomic targets**

M. Yáñez **On the existence and lifetimes of complexes between neutral systems and indications**

R.D.Rivarola **Coherent electron emission from molecular targets**

P.D. Fainstein **Photoionization of the hydrogen molecular ion: angular distributions and interference effects**

GAS–SURFACE DYNAMICS

R. Olsen **Why rough surfaces make good catalysts—reaction mechanisms of hydrogen on the Pt(211) stepped surface**

R. Sayós **DFT and classical dynamics study of atomic oxygen interaction on ?-cristobalite (100)**

G.-J.Kroes **The electronically adiabatic approach to diffractive and reactive scattering of H2 from metal surfaces**

A. Gross **Adsorption dynamics at surfaces including energy transfer to the substrate**

C. Díaz **Dissociative chemisorption of N2 on Ru(0001)**

A. Salin **Structure—reactivity relation in N2 dissociation on W surfaces**

GAS–SURFACE DYNAMICS

P. Rivière **Interaction of H2 and D2 with NiAl(110)**

W. Dong **Solute transfer from micelles to a bilayer adsorbed on a hydrophilic solid surface**

ELECTRON DYNAMICS

D. Vernhet **Dynamics of laser-cluster interaction probed by X-ray spectroscopy**

J.-P. Gauyacq **Core-excited Ar*(2p-13/2 nl) atoms in various environments: surfaces and bulk**

D. Sánchez-Portal **Charge transfer at surfaces: the case of Ar and S on Ru(0001)**

CHEMICAL REACTIVITY

J.C. Rayez **The statistico-dynamical approach: a transition state theory revisited**

P. Larrégaray **Validity of phase space theory for atom-diatom insertion reactions**

L. Bonnet **Gaussian weighting in the quasiclassical trajectory method**

GAS–SURFACE DYNAMICS

V. Sidis **The interaction and recombination of H atoms at a graphite surface**

M. Rocca **Role of rotational alignment in gas-surface interactions and simple chemical reactions**

F. Martín **Diffraction and reactivity of H2 molecules on Pd surfaces**

V. H. Ponce **Concluding remarks**

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