DONOSTIA INTERNATIONAL PHYSICS CENTER

Reporting on 2002/03

How to see the 3D illusion

Hold the image close to your face and slowly pull it away. Look through the image without focusing on it. Stop at a reading distance and try not to blink. E Acercar la imagen a la cara, alejándolo lentamente. Intentar mirar la imagen sin enfocar. Parar a la distancia de lectura sin pestañear. EH **Irudia aurpegira hurbildu, pixkanaka aldenduz. Saiatu fokatu gabe begiratzen. Irakurtzeko tartean geratu kliskatu gabe.** SF Laita kuva lähelle kasvojasi ja työnnä sitten hitaasti kauvemaksi katsoen kokokuvaa. Pysäytä ja katso räpyttämättä silmiä. F **Tenir l'image près du visage et l'éloigner lentement. Essayer de regarder à travers sans cligner des yeux.** I Avvicinare la immagine al viso, allontanandola lentamente. Cercare di guardare la immagine senza focalizzare. Fermarla alla distanza idonea per la lettura e non sbattere le ciglia. SE **Håll bilden några centimeter från ditt ansikte och flytta den sakta ut. Titta igenom bilden utan att fokusera på den. Håll den på läsaustand och försök att inte blinka.** प्रतिबिम्ब को अपने चेहरे के नजदीक रखें और फिर धीरे – धीरे उसे अपने से दूर ले जायें। अपना यान प्रतिबिम्ब पर केन्द्रित किये बिना उसमें देखते रहें। और बिना पलक झपकाते हुये स्पष्ट पढ़ने की दूरी पर जा कर रूके। D **Halten Sie das Bild nahe an Ihr Gesicht. Während Sie den Abstand langsam vergrössern, schauen Sie das Bild an ohne zu fokussieren. Halten Sie es in normalem Leseabstand und versuchen Sie, nicht zu blinzeln.** Приблизить изображение к лицу. Затем медленно начать его отодвигать, пытаясь смотреть на него без фокусировки. Остановиться на расстоянии чтения без моргания.

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Reporting on 2002/03

THE TASK IS,

NOT SO MUCH TO SEE
WHAT NO ONE HAS
YET SEEN;
BUT TO THINK
WHAT NOBODY HAS
YET THOUGHT,
ABOUT THAT WHICH
EVERYONE SEES.

Erwin Schrödinger

INSIDE Reporting on 2002/03

Pedro Miguel Echenique Landiribar President

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.

WELCOME
TO THE DIPC FOUNDATION

Present and Future

The 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.

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 ▸

Pedro Miguel Echenique Landiribar is Professor of Condensed Matter Physics at the University of the Basque Country. He obtained his PhD at Cambridge (1976) and Barcelona (1977) and has Honorary degrees from Cambridge (Doctor of Science 1998) and Doctor Honoris Causa from Valladolid (2000). He is a Fellow of the American Physical Society (FAPS) and of the American Association for the Advancements of Science (FAAAS). He is recipient of Prince of Asturias of Scientific Research Prize, Max Planck Physics Prize, Euskadi Prize of Investigation, Iberdrola Prize of Science and Technology, Gold Medal of the University of the Basque Country and of the City of San Sebastian, Great Cross of Alfonso Xth El Sabio.

Juan Colmenero de León General Director

In this short period, DIPC has become a center of reference in basic research of Materials Physics.

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

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 since a person will not be considered educated without some basic knowledge of scientific and technical issues.

After four years, we can say that the objectives we set from the start have been accomplished. In this short 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, 2002-03, 187 original papers have been published in journals such as, Physical Review Letters (21 papers) and Physical Review (55 papers). This means that the contribution in 2002-03 from DIPC in these journals is in the order of 8% 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 first stage of 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.

Juan Colmenero de León is Professor of Condensed Matter Physics at the University of the Basque Country. He obtained his PhD in Physics by the University of Navarra (1979). His research activities are Polymer Physics and Non-Crystalline Materials. He is a member of the Editorial Board of the Journals: Colloid & Polymer Science (Springer) and Journal of Polymer Science B, Polymer Physics (WILEY). He is also Chairman of the Selection Panel of the European Project "Jülich Neutrons for Europe" and Spanish representative at the Advisory Committee of the Institute Laue Langevin (ILL, Grenoble). He has been awarded the "Xabier María de Munibe" Prize in Science & Technology (1998) given by the Basque Parliament and the Euskadi Prize of Research in Science & Technology (2000) given by the Basque Government.

Alberto López Basaguren Secretary

We hope that the new computation center will become one of the basic pillars for future developments of scientific activity at DIPC through continuous updates in hardware.

The principal objective in this second stage of development is the creation of a critical mass of staff researchers at DIPC.

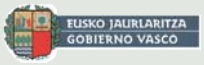
In addition to DIPC scientific level, it is also gaining recognition internationally as a center of innovation, as other universities and research centers have recently shown interest in our model of operation.

Spurred by these remarkable results after our initial launching stage, we now face the challenge of developing DIPC into a powerful center for basic research. Along the same line, we can include the creation of our new in-house Computation Center. This center arose with the aim of becoming an international reference in complex computational physics and materials simulation. 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.

The principal objective in this second stage of development 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, we have started a new 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.

The deployment of these programs also requires a substantial increase in the budget of the Foundation. In addition, new spaces will have to be made available, which will involve the refurbishment of the fourth building at the DIPC premises. ■

Alberto López Basaguren is Professor of constitutional law. He obtained his degree in political sciences from Universidad Complutense in Madrid and PhD from the University of the Basque Country (1990). He furthered his studies in Florence and Bologna (Italy). He continues his research in economic, constitutional and linguistic law and its integration in the European Community. He is formerly Secretary General of the University of the Basque Country.



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

Provincial Authority of Gipuzkoa

Gipuzkoako Foru Aldundia
Diputación Foral de Guipuzcoa

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Donostiako Udala
Ayuntamiento de San Sebastián

Kutxa

Iberdrola

OUR PATRONS

The Board is the principal governing body of the DIPC Foundation.

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NEW SPACE

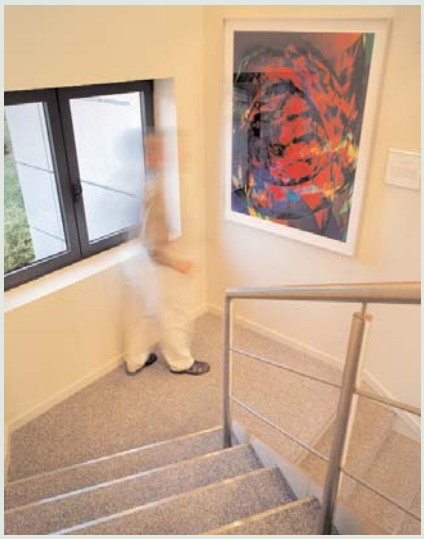
The Opening of the DIPC Computation Center

Patrons and board members examine the first installed units at the opening of the Computation Center.
From left to right: Joseba Jaureguizar, José Ramón Guridi, José Ignacio Telletxea, Juan Colmenero, Fernando Cossío, Jon Ramón Beloki, Alfredo Zalaia, and Alberto López Basaguren.

One of the priorities of Donostia International Physics Center is the development of basic research in materials science at the highest level. Within this line, DIPC relies on complex computational calculus and simulation methods as basic tools. The developments in this science advance towards complexity and towards multi-component, nano-structured and biological materials. It is widely accepted that modern computation and simulation methods, along with the future development of computers, will be indispensable in this field. DIPC intends to develop multi-scale calculation and simulation methods, which are appropriate for the study and modeling of materials. The scope of the fields covered ranges from the electronic and atomic scale ("*ab-initio*" methods) as well as molecular, nanometric and mesoscopic scales.

The first phase of the new DIPC Computation Center was inaugurated at DIPC in July 2003. The institute's own calculation center is connected to the general service of the University of the Basque Country (UPV/EHU) and is optimized for computational and simulation purposes in materials science. This center operates with an open layout, which will allow for new modern methods, such as intensive distributed and interconnection calculus to be carried out with other international computation facilities. This however will require the constant deployment of adequate up-to-date computational hardware. ■

The new DIPC Computation Center affords the opportunity for Basques and DIPC's visitors to access a facility with state-of-the-art calculating power.



Patrons of the DIPC Foundation, from left to right: Juan Colmenero, Anjeles Iztueta, Pedro Miguel Echenique, Josu Jon Imaz and Alberto López Basaguren.

The development of this center will require the constant deployment of adequate up-to-date computational hardware.

Odón Elorza, José Ignacio Telletxea, Fernando Cossío, Juan Colmenero and Félix Ares.

RESEARCH ACTIVITY

DIPC is dedicated to two main areas of research.

Condensed Matter Physics

The current activity —mainly theory and computational physics— is focussed on four different lines: Theory of Scanning Tunneling Microscopy, Interactions of ions with matter; Electronic response of surfaces, solids and nanostructures; Interaction of fast electrons and radiation with nanostructured materials. Moreover, a Nano-Physics Laboratory project is being developed in collaboration with a Technological Center of the Basque Country (Labein). Within these general areas, different recent topics can be identified:

Interaction of ions with matter

Phase effect in the stopping of ions in metals
Stopping of slow ions in insulators

Electronic response of surfaces, solids and nanostructures

Dynamics of electrons and holes in solids and at their surfaces
Electronic properties in finite and extended systems
Electronic structure and magnetic properties of nanowires

Interaction of fast electrons and radiation with nanostructured materials

Interaction of radiation and fast electrons with complex nanostructures (Smith-Purcell and microscopy based light emission induced by fast electrons)
Plasmon excitations in nanostructures
Photoemission from core and valence levels

Polymers and Non-crystalline Materials

The current activities in this area are focussed on the general line: Molecular motions and relaxation processes in polymer materials and glass-forming systems. This is mainly an experimental approach by combining different techniques, in particular, neutron scattering, broadband dielectric spectroscopy and NMR. Moreover, we are also developing fully atomistic molecular dynamics simulations of polymer systems. Within this general area, we can identify the following recent topics of research:

Molecular motions and relaxation processes in polymer materials and glass-forming systems

Dynamics of multicomponent polymer systems

Atomistic MD-Simulations in polymers

Dynamics of glass-forming polymers and the problem of the Glass Transition

Relationship between transport properties and molecular mobility in polymeric membranes

Microscopic understanding of relaxation processes in engineering thermoplastics

SCIENTIFIC HIGHLIGHTS

Index

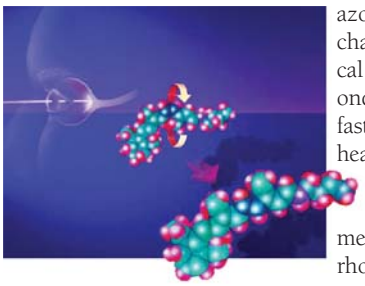
DIPC Highlight

Understanding Biological Photoreceptors

by *M.A.L. Marques[1], X. López[2], D. Varsano[1,3], A. Castro[4,3] and A. Rubio[1,3,5]*

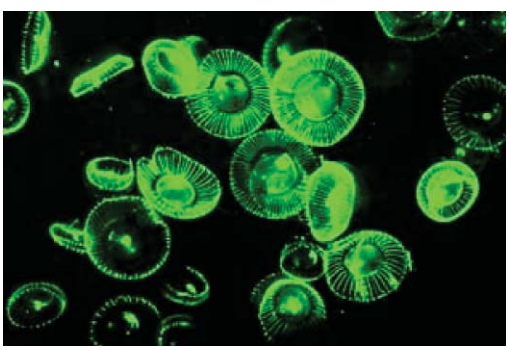
We have implemented a new scheme to describe the photoresponse and structural dynamics of bio-photoreceptors. The scheme can shed light into the initial microscopic origin of vision, photosyntesis and bacteria luminiscence processes.

Chromophore isomerisation is at the heart of biomolecular photophysics.

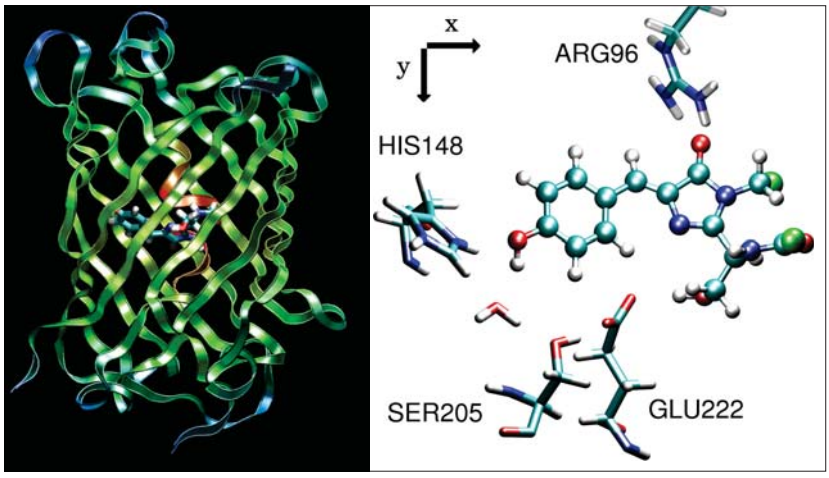


One of the most fundamental, intriguing and relevant bio-physical process is the microscopic description of the photo-response of bio-molecules. From the photosynthesis to the human vision processes, DNA damage and bacteria bio-luminescence; those phenomena require an understanding of how light is absorbed and how that energy is transfer from the photoreceptor sites to the active biological centers. A famed organic molecule is the azobenzene chromophore, (formed by joining two phenyl rings with the azo group) that undergoes a structural change (cis/trans-isomerization) under optical irradiation, and it does so in a femtosecond time-scale. These light-induced ultra fast rotations around double bonds are at the heart of most photo-active bio-organic reactions. In particular the first step of the human vision are related to cis/trans isomerization of the retinal chromophore of rhodopsin (see figure). The induced structural transformation upon light absorption is very fast (few hundred femtoseconds; 1fs=10^{-15}s) and is associated to the presence of ring structures in the molecule (as benzene or imidazoline groups).

The cited phenomena involve i) different energy (from covalent to van der Waals bonding) and time scales (from fs for the electron dynamics, to ps for the ionic motion and ms for structural reorganizations); ii) light-induced chemical reactions that are intrinsically non-adiabatic, and require techniques that go beyond the traditional Born-Oppenheimer separation of electronic and nuclear degrees of freedom. Therefore, there is a clear need for a reliable theoretical framework to describe processes related to the excited-state dynamics of biological complexes either in vacuo or in solution. In 2002 we joined efforts with the theoretical quantum chemistry group to set up an ambitious project with the goal of developing a theoretical scheme able to predict the photo-induced dynamics in bio-molecular structures. We present here the first results noticing that many other fascinating results are just coming up. Our approach is based on a divide-and-conquer strategy where the active part of the structure is fully described microscopically using quantum mechanics schemes, whereas the environment (i.e., rest of the protein, membrane and solvent) is described using a classical molecular mechanics method (QM/MM approach). The novelty of our work is the simulation of the combined electron-ion dynamics of the photoreceptor within the framework of time-dependent density functional theory (TDDFT). By solving a set of coupled time-dependent Schrödinger-like equations (including light sources as short laser pulses), we identify the mechanisms active at the different time-scales of the photo-process.



1 Departamento de Física de Materiales, UPV/EHU, San Sebastián, 2 Departamento de Química, UPV/EHU, San Sebastián, 3 Donostia International Physics Center, San Sebastián, 4 Departamento de Física Teórica, Universidad de Valladolid, Spain, 5 Centro Mixto CSIC-UPV/EHU, San Sebastián



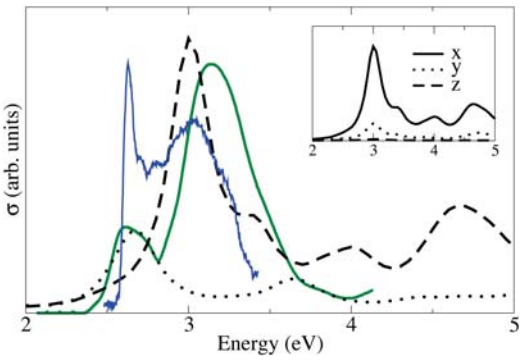
In this context, the Green Fluorescent Protein (GFP) has become a unique tool in molecular biology because of its fluorescent properties and inertness when attached to other proteins. The optical absorption spectrum of the wild type (wt)-GFP, measured at 1.6 K, shows two main resonances at 2.63 and 3.05 eV that are attributed to the two thermodynamically stable protonation states of the chromophore (negative and neutral configurations, respectively). Excitation at either frequency leads to fluorescent green-light emission, peaked at 2.44eV, which is the main mechanism for energy release in wt-GFP. This internal photo-conversion process occurs very rapidly by excited-state proton transfer for the neutral chromophore. The photo-physics of the GFP is governed by a complex equilibrium between the neutral and anionic configurations. Thus, GFP is the ideal system to test our theoretical approach. First we determined the structure of the GFP and then computed the photo-absorption cross section for visible light as it has to be properly described before we could dream of describing any dynamical process.

The GFP protein is folded in a b-sheet barrel conformation with the cromophore occupying a central position inside the barrel (see figure). The cromophore is formed by two consecutive rings, the phenol-type ring of Tyr66 and a five member heterocyle formed by the backbone of Tyr66, the carbonyl carbon of Ser65 and the nitrogen of the backbone of Gly67. The theoretical photo-absorption cross-section is compared to the experiments in the figure (the dashed line corresponds to the neutral chromophore, the dotted line to the anionic, whereas the green and blue curves are the experimental results of S.B. Nielsen et al, PRL87, 228102 (2001) and of T.M.H. Creemers et al, PNAS 97, 2974 (2001), respectively). The strength of the main p - p* transition is larger in the anionic than in the neutral GFP. It is, however, possible to obtain a quantitative description of the spectra of the wt-GFP by assuming a 4:1 ratio for the concentration of the neutral/anionic forms. This value is very close to the estimated experimental ratio of 80% neutral and 20% anionic. Besides the good description of experiments we noticed that GFP is a rather anisotropic molecule in the visible (see inset in the figure). Only light polarized along the pentagon-hexagonal ring is absorbed with high yield. This property can be used to enhance the photo-dynamical processes of GFP samples for opto-electronic devices, e.g. depositing well oriented GFP molecules on top of doped-semiconductor substrates we could get photovoltaic structures with high efficiency.

We have shown that a combined QM/MM and TDDFT approach is able to reproduce the optical response of the GFP. This is a major step toward the first-principles description of excited-state dynamic of important biological photo-receptors. Transient and time-resolved optical spectroscopy could be studied. However, in spite of the good agreement, some questions remain open. For example, how does the excitation in the GFP trigger the proton shuttle mechanism and what is the time-scale for this process? To answer these questions we have to go beyond the present work including the excited state dynamics of the environment (e.g. the proton-transfer involves structural modifications of the environment that have to be properly described). Work along this line is in progress. ■

Our TDDFT approach constitutes a major step towards the first principles description of the combined electron/ion dynamics in bio-photoreceptors.

REFERENCE
M.A.L. Marqués, X. López, D. Varsano, A. Castro and A. Rubio, Physical Review Letters **90**, 258101 (2003)



DIPC Highlight

Mixing One-dimensional Cold Atomic Gases

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

Just as mixing two fluids (e.g. water and oil) under certain conditions of temperature and pressure can lead to a variety of phenomena, mixing two types of cold atomic gases confined to one-dimension can lead to a number of interesting quantum phenomena. This includes the usual demixing (like the one observed at room temperature and pressure between oil and water), collapse, or more interestingly the formation of "pairs" of atoms of different species that are correlated over long distances.

The large tunability of cold atomic gases allows to study interesting many body phenomena.

Ever since the achievement of Bose-Einstein condensation of a dilute gas of alkali (Rubidium) atoms in the summer of 1995, the field of cold atomic gases has made astonishing experimental progress. The ultimate goal has become to learn how to manipulate cold atomic gases to realize exotic phases of matter. The latter may find applications in quantum information processing and storage. It is also expected that they can provide us with new and key insights into the physics of quantum many-body systems that may help us understand some of the puzzling behaviour of the high-Tc copper-oxide superconductors and other exotic materials.

One dimensional systems of cold atoms have only recently become available, and are very interesting because of the strong enhancement of correlations as the dimensionality of the system decreases. So far, most experiments are made with bosonic atoms (like ^{87}Rb) confined by very anisotropic potentials. However, not far in the future fermions (like ^{6}Li) will also be used. Bosons confined to one dimension (1D) are interesting per-se, as there are not many realizations of these systems in Nature (apart from spins in highly anisotropic magnetic materials).

A single-component gas of cold bosons, when confined to 1D, will not undergo Bose-Einstein condensation since all possible fluctuations must propagate on a line and any kind of ordering (like Bose-Einstein condensation) will be strongly suppressed. However, in the finite-size systems of experimental interest, phase coherence can be approximately maintained over many times the average atom-atom distance so that these systems resemble very much a Bose-Einstein Condensate (BEC). This is why they are frequently called quasi-condensates. However, if the strength of the interactions is increased, the (phase) fluctuations are enhanced and the system will not behave as a condensate anymore. This is the case as the extreme limit where no boson can pass each other (i.e. the bosons become "hard core") is approached. A gas of hard-core bosons is known in the jargon of the field as a Tonks gas, in honor of Lewi Tonks, who first discussed the properties of a classical gas of hard-core particles in 1936. Between the Tonks gas limit and the quasi-condesate, the system exhibits a rather smooth crossover, and no new phenomena are expected.

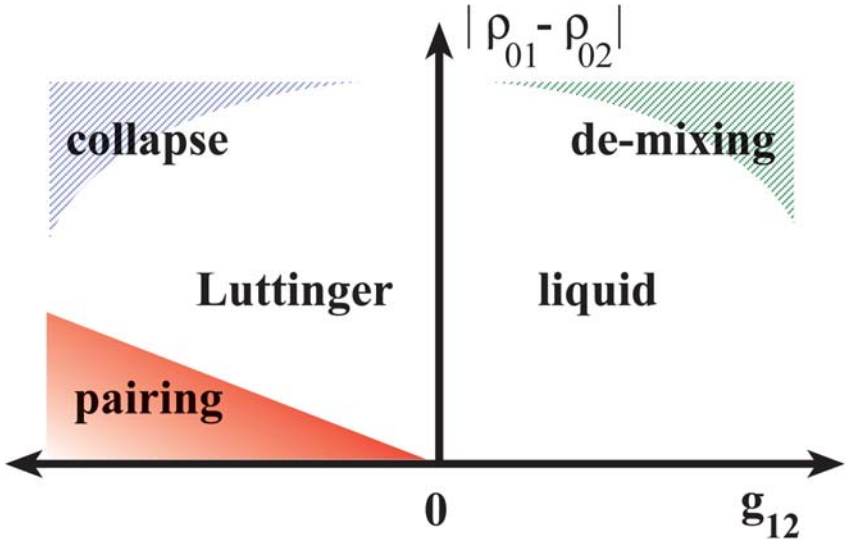
On the other hand, when a two-component 1D gas is considered (a binary mixture), the

1 Donostia International Physics Center, San Sebastián 2 School of Physics and Astronomy, University of Birmingham, Edgbaston, U.K.

resulting system exhibits a much richer and interesting behaviour. First of all, just like with ordinary (classical) fluids, the system can demix (like oil and water do at room temperature and pressure) if the two components repel sufficiently strongly, or it can collapse if they attract sufficiently strongly. However, the quantum nature of this matter leaves room for more surprises.

In 1974 two American theoretical physicists stumbled upon a particular type of one-dimensional matter. When opposite-spin electrons attract in a one-dimensional metal they could form pairs. The analogy with the so-called Cooper pairs, discovered by Leon Cooper in 1957, and which eventually would be instrumental for understanding the mechanism of superconductivity in conventional superconductors (like lead or aluminum), was unavoidable. However, as Luther and Emery cleverly pointed out, fluctuations would never allow the electron-pairs to condense (as Cooper pairs do in superconductors), and therefore establish a macroscopic phase coherence throughout the system. That is why the system would exhibit a gap only to spin excitations and would remain gapless for charge excitations. In contrast, in higher dimensional materials condensation of Cooper pairs opens a gap to all excitations, both spin and charge, and only in neutral systems (like in Helium 3) one can have a gapless collective mode known as the Anderson-Bogoliubov mode. All in all, the model was the closest thing to a higher dimensional superconductor that one can get in one dimension, and it goes under the name of Luther-Emery liquid.

Remarkably, we found that the phenomenon discovered by Luther and Emery can also take place in a binary mixture of two cold atomic gases. In our letter, we studied two types of these systems, depending on the statistics of the components. Thus if the two components are bosonic, we termed the mixture of B+B type, whereas it one of the components is a boson and the other is a fermion, we termed it of B+F type. We found that if the bosons of the same type repel each other very strongly, i.e. if they are driven into the Tonks gas regime, and provided the number of particles of each species and the velocity are equal and different species attract, they could form the same type of pairs that Luther and Emery found for a one-dimensional metal where electrons attract each other.



Schematic phase diagram with the boson(s) in the Tonks limit. $|\rho_{01} - \rho_{02}|$ is the density difference

In a mixture of a boson and a fermion, this has interesting consequences, the pair (the "composite fermion") will behave as a fermion and therefore carries a finite momentum which is of the order of the Fermi momentum. This is somewhat analogous to the condensation of Cooper pairs at finite momentum that takes place in certain superconductors under the influence of a strong magnetic field (the so-called Fulde-Ferrell-Larkin-Ovchinnikov state). However, the analogy cannot be pushed too far, because in contrast to the latter systems, the composite fermions would never condense even in higher dimensions due to their statistics. In 1D however, for sufficiently strong attraction between the boson and the fermion, the gas of composite fermions would still acquire some superfluid properties. ■

We have found an exotic phase where atoms of two difference species pair up in a strongly correlated cold atomic gas confined to move in one dimension

REFERENCE
M. A. Cazalilla and A. F. Ho, Physical Review Letters **91**, 150403 (2003)

DIPC Highlight

Role of Bulk and Surface Phonons in the Decay of Metal Surface States

by *A. Eiguren[1], B. Hellsing[2], F. Reinert[3], G. Nicolay[3], E. V. Chulkov[1,4], V. M. Silkin[4], S. Hüfner[3] and P. M. Echenique[1,4]*

Understanding the temporal evolution of quasiparticles (electron and holes) on metal surfaces is of paramount importance to describe many important phenomena such as the dynamics of charge and energy transfer, quantum interference, and localization. Typically, the quantity used to characterize this temporal evolution is the lifetime, which refers to the time the quasiparticle retains its identity. It is the interaction of the quasiparticle with the metal (electrons, phonons...) what makes the lifetime finite. We present the first microscopic analysis of the electron-phonon mechanism and find that its contribution, together with the electron-electron mechanism, is crucial in order to understand the experimental lifetime of the sp surface state on Cu (111) and Ag (111).

Electron-phonon interaction gives important contribution to electron (hole) dynamics on metal surfaces and controls temperature dependence of this dynamics.

The sp surface state in the L-gap of the (111)-surface of noble metals forms a two-dimensional (2D) electron gas and the electron-electron (e-e) contribution to the hole lifetime has been rationalized in terms of a dominant contribution from intraband transitions within the 2D surface state band, screened by the underlying 3D bulk electron system, and in terms of interband transitions (bulk states $\rightarrow$ surface state) (Science, 288, 1399 (2000)). However, an appropriate calculation of the electron-phonon (e-p) contribution to the lifetime broadening of surface states has not been done yet. Many properties of metals, such as resistivity, specific heat, and superconductivity, reflect the importance of the e-p interaction. The strength of this e-p coupling is usually measured in terms of a parameter λ that depends on the energy and momentum involved in the process under consideration. We have presented a theoretical analysis of the e-p contribution to the lifetime broadening of surface electron states, taking into account all electron and phonon states involved in the e-p scattering process. The theoretical analysis is based on a calculation of the full Eliashberg spectral function, which enables us to resolve, in detail, the contributions from different phonon modes, as well as, the general temperature dependence. Including the e-e interaction, our theoretical results are compared with new energy and temperature dependent high-resolution photoemission data.

In Fig.1 the calculated temperature dependent e-p contribution (solid lines) to the lifetime broadening Γ together with e-e contribution Γ_{ee} (dotted lines) is compared with the measured temperature dependence of Γ (circles) for Cu (111) and Ag (111). The insert shows the measured energy distribution curves for Cu (111) for selected temperatures.

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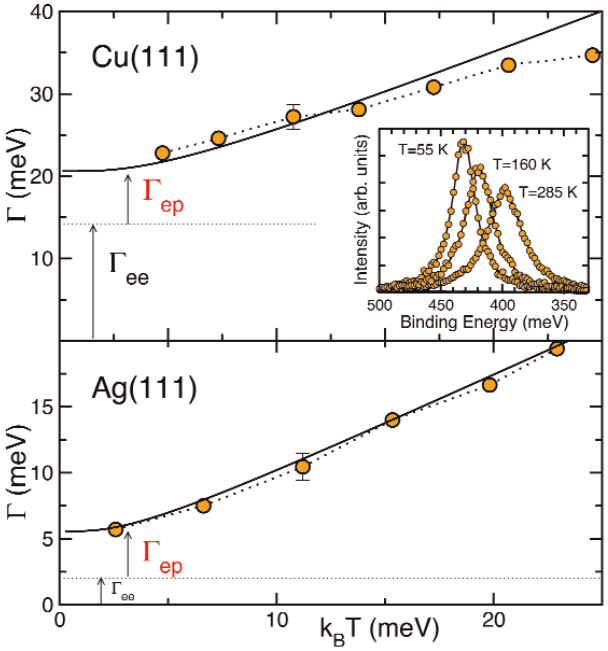

Fig.1. Temperature dependence of the lifetime of the sp surface state

Surface phonon modes are crucially important for the description of electron dynamics on surfaces.

In Fig.2 the calculated Γ_{ep} (red lines) as well as Γ_{ee}+ Γ_{ep} (black lines) are shown for Cu (111) and Ag (111) together with the experimental results (diamonds) as a function of energy at T=30K. As follows from Fig. 2, the contribution from only the Rayleigh mode (blue lines) gives about 40% of Γ_{ep} beyond the maximum phonon frequencies, indicating that bulk phonons give most of the contributions in this range. But for binding energies below the maximum of the Rayleigh mode energy, this mode alone represent on average about the 85% of Γ_{ep}.

Detailed comparison of the theoretical results with photoemission data (this work and Phys. Rev. B 63, 115415 (2001)) as well as with scanning tunnelling spectroscopy results (Science, 288, 1399 (2000)) shows an excellent agreement between the theory and experiments that opens new perspectives in investigations of dynamical processes on clean metal surfaces as well as on surfaces with adatoms and adlayers at different temperatures. ■

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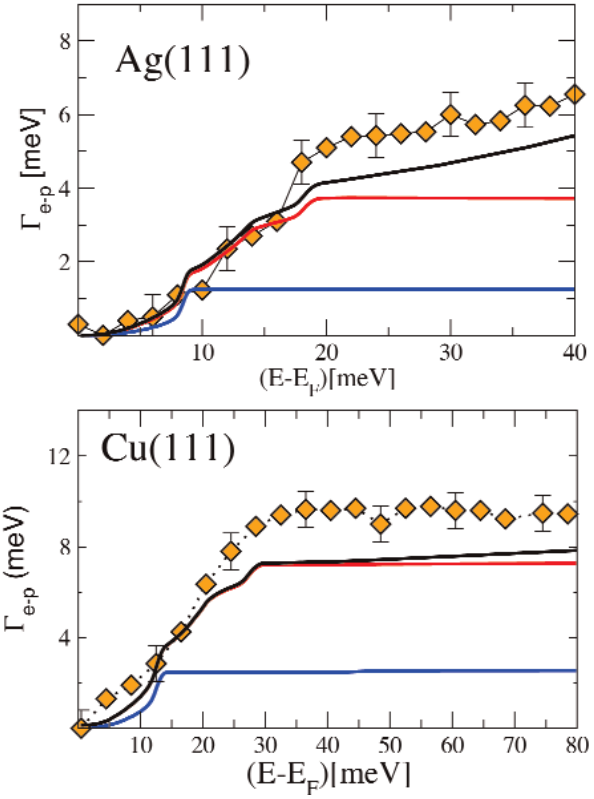

Fig. 2. Lifetime broadening of the electron state depending on its binding energy

DIPC Highlight

Cherenkov Effect in Photonic Crystals

by *F. J. García de Abajo*[1], *A.G. Pattantyus-Abraham*[2], *N. Zabala*[1,3], *A. Rivacoba*[1,4], *M.O. Wolf*[2], *and P. M. Echenique*[1,4]

Like the wake produced by a boat moving faster than surface waves in a quiet lake, fast electrons moving faster than light in a dielectric produce the so-called Cherenkov radiation, which leads ultimately to stopping of the projectiles.
This effect has been observed for electrons traversing photonic crystals, where light is subject to a periodically modulated dielectric constant and allowed to propagate within so-called photon bands, similar to electronic bands in solids. The electrons lose energy to produce photons with probability proportional to the local density of the photonic states at the position of the electron beam. This permits us to map photonic bands by observing the energy and angle distribution of the transmitted electrons.

Cherenkov light can reflect how photons propagate in photonic crystals.

Light can be slowed in matter so that charges traveling faster that it may lose part of their energy to produced a cone of Cherenkov light emission, similar to the wake of a boat moving faster than surface waves in water. The same phenomenon can take place if the charges move inside a photonic crystal, where light is subject to propagation only along certain directions for given frequencies, and the resulting light emission must reflect the complexities of the photonic band structure in these materials.

Our group, working in collaboration with Dr. Andras Pattantyus and Dr. Michael Wolf of the University of British Columbia (Canada), have managed to prove this effect by observing energy losses in fast electrons transmitted through pores drilled in 1-micron thick alumina films. The transmitted electrons exhibited a marked tendency to lose energy in the 7-8.5 eV region, depending on the velocity of the electrons and in good agreement with calculations of light emission proba-

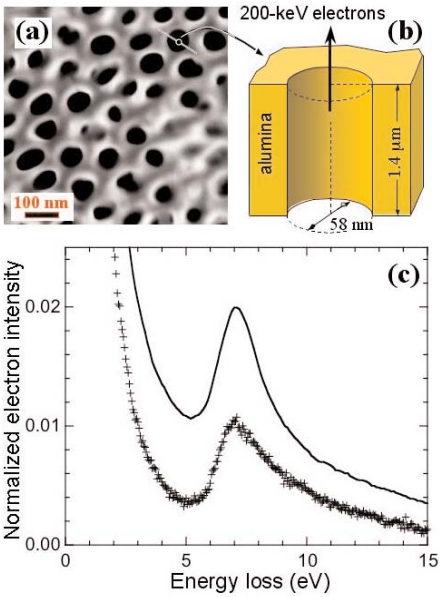

Fig. 1. Cherenkov losses in a photonic crystal

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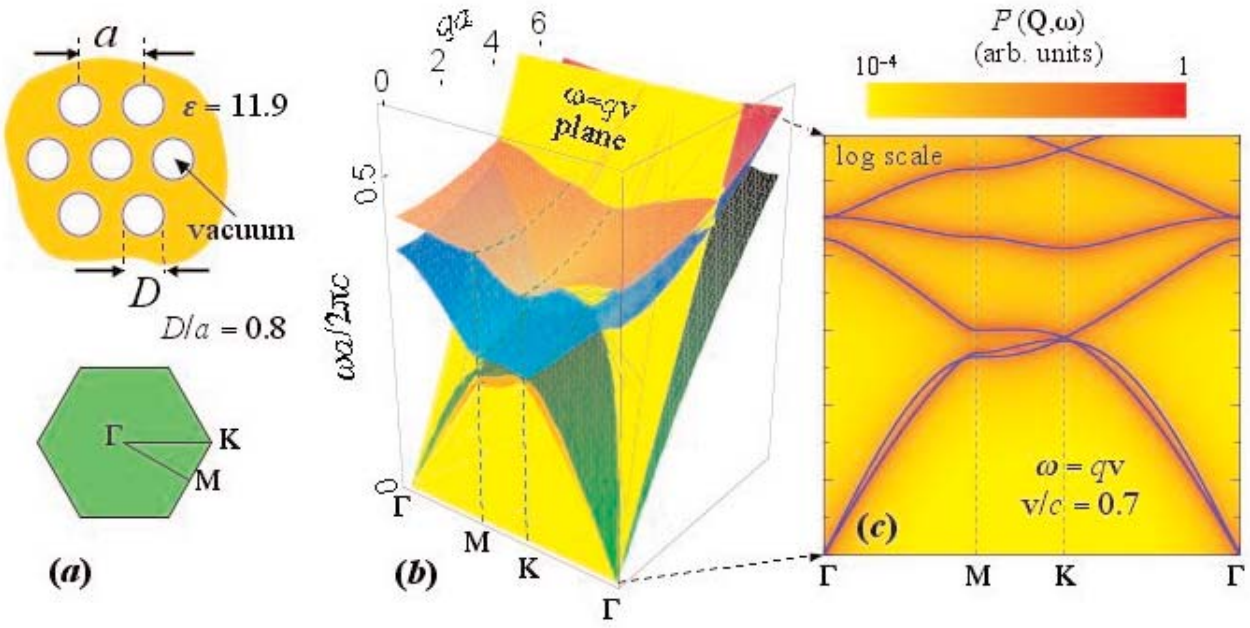

Fig. 2. Mapping photonic bands with fast electrons

bility, which is more pronounced at those energies. The electrons were made to pass through the holes without actually touching the material, and the fact that alumina is transparent across distances of several microns at those photon energies led the researchers to conclude that the observed energy losses must arise from Cherenkov light emission. More precisely, Fig. 1 shows a transmission electron microscope image of a porous alumina film (a), a schematic view of one of the holes showing the electron trajectory (b), and the distribution of electrons as a function of the energy that they have lost (c), theory (symbols) compared with experiment (curve), with clear evidence of the Cherenkov effect (7 eV peak).

Unlike Cherenkov emission in a homogeneous medium, the restriction imposed by a 2D patterning of holes in the alumina films limited this emission to within the abovementioned energies. Further analysis of the bending in the trajectory of the electrons can provide a basis for direct mapping of photonic bands by fast electrons, theory suggets (see Physical Review Letters 91, 143902, 2003), as shown in Fig. 2, that depicts a schematic diagram of a two-dimensional crystal made of cylindrical holes, along with its first Brillouin zone (a), the band structure of this crystal and its variation with light momentum parallel to the cylinders q (b), and a cut of the bands along the **ω=**qv plane (c). Electrons moving with velocity v along the cylinders can only sense photonic states that satisfy this condition. The underlying density plot in (c) shows the probability that the electrons lose a certain amount of energy w with their trajectory is deflected by a given momentum within the first Brillouin zone. ■

Photonic bands are mapped by energy and angle distributions of fast electrons transmitted through photonic crystals.

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DIPC Highlight

Interplay of Surface Plasmons and Image States

by *A. García-Lekue[1], J.M. Pitarke[1,2], E.V. Chulkov[2,3], A. Liebsch[4] and P.M. Echenique[2,3]*

Our investigations on the combined effect of single-particle and collective surface excitations in the decay of image-potential states on Ag surfaces provide new insight to elucidate the origin of the long-standing discrepancy between experimental measurements and previous theoretical predictions for the lifetime of these states. Although surface-plasmon excitation had been expected to reduce the image-state lifetime, we have demonstrated that the subtle combination of the spatial variation of s-d polarization in Ag and the characteristic non-locality of many-electron interactions near the surface yields surprisingly long image-state lifetimes, in agreement with experiment.

The coupling of excited states with the solid governs the cross sections and branching ratios of practically all electronically induced adsorbate reactions at metal surfaces.

Fundamental concepts in condensed matter physics are those of surface plasmons and image states. Surface plasmons, which are quanta of collective oscillations of electrons at metal surfaces, crop up in a number of scenarios from electron energy loss to the colourful appearance of suspensions of small metallic particles, surface-plasmon resonance technology, and a wide range of photonic applications. Image states are quantized electronic states that are observed outside certain metal surfaces due to the attractive image potential that occurs between the electron and the solid. Image states dynamics provides insight into the investigation of the coupling of excited surface electronic states with the underlying substrate. This coupling of these states with the underlying substrate is known to govern the cross sections and branching ratios of practically all electronically induced adsorbate reactions at metal surfaces.

In most metals, there is no interplay between surface plasmons and image states, which is due to the fact that the surface-plasmon energy is typically too large for image states to couple with them. In silver, however, the presence of occupied narrow bands of d electrons considerably reduces the surface-plasmon energy, and the relaxation of image states via the creation of surface collective excitations becomes feasible in this material.

The broadening (and therefore finite lifetime) of the first (n=1) image state at the Γ point on the Ag(100) surface mainly originates in processes in which the image-state electron with an energy of 3.9 eV above the Fermi level decays into an empty state with energy still above the Fermi energy. These processes can be realized by transferring energy and momentum to an excitation of the medium, thereby creating either an electron-hole pair or a collective surface excitation of energy smaller than 3.9 eV. The energy of surface plasmons in Ag is 3.7 eV.

The inelastic broadening of excited states in solids can be obtained from the projection (over the excited state wavefunction) of the imaginary part of the so-called electron self-energy of many-body theory, which accounts for the many-body interactions in the solid. Following this formalism, we have investigated the decay of the Ag (100) n=1 image state by treating Auger-like single-particle and collective surface excitations on the same footing. A consistent treatment of these decay channels is particularly important because of the near-degeneracy of the image state energy with the Ag (100) surface plasmon.

The surprising and novel result of our work is that, although the imaginary part of the image-state self-energy is enhanced due to the presence of the plasmon decay channel, interferences resulting from the non-locality

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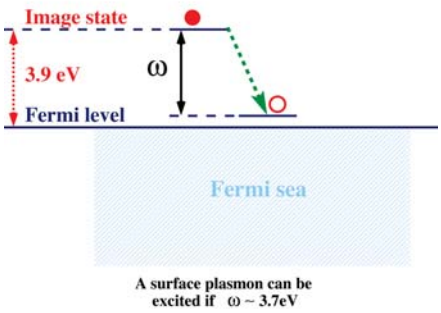

Energetic diagram of the decay of the first Ag (100) image state

of the self-energy lead to a smaller overall image-state broadening, in agreement with experiment. This elucidates the origin of the long-standing discrepancy between experimental measurements and previous theoretical predictions for the lifetime of these states.

First-principles descriptions of electron dynamics in the bulk of noble metals show that deviations from electron dynamics in a gas of sp electrons mainly originate in the participation of d electrons in the screening of electron-electron interactions. Hence, in order to avoid the use of too-expensive ab initio techniques at the noble metal surface Ag (100), the approach we have undertaken is based on (i) the use of a physically motivated one-dimensional potential which accurately accounts for the dynamics of sp valence electrons, and (ii) the replacement of occupied d bands in Ag by a polarizable medium giving rise to additional screening. We emphasize that our approach provides a coherent treatment of single-particle and collective surface excitations.

The n=1 image-state wave function on Ag (100) (dotted line in the figure, where z is the coordinate normal to the surface) has a maximum at a few angstroms outside the crystal edge (z=0), which we choose to be located half a lattice spacing beyond the last atomic layer. The solid line in the figure shows the imaginary part of the n=1 image-state self-energy (this nonlocal quantity Im[-Σ] couples the coordinates z and z') versus z for a fixed value of z' outside the solid (red circle). We note that the main peak of Im[-Σ] does not occur at z=z', as would be the case in the interior of the solid; instead, it lags behind and remains localized near the surface where the image-state wave function is negative. Consequently, there is a major interference contribution to the projection of Im[-Σ] over the image-state wave function, which is negative and yields a large reduction of the image-state broadening.

The role that the screening of d electrons plays lowering the surface-plasmon energy, and therefore opening a new coupling of image states with the solid, is particularly pronounced on the vacuum side of the surface, where negative interference dominates. Hence, the combined effect of decay via surface plasmons and nonlocality of the self-energy is a considerably reduced lifetime broadening. While in the absence of d electrons the broadening of the n=1 image state on Ag (100) would be 18 meV, our theory (with d electrons and surface-plasmon decay included) yields a broadening of 12 meV (i.e., a lifetime of 55×10^{-15}s) in excellent agreement with recently reported time-resolved two-photon photoemission (TR-2PPE) measurements. ■

Despite the enhancement of the image-state self-energy in Ag due to the decay via surface plasmons, the highly nonlocal character of the self-energy in the surface region ultimately leads to a surprisingly small lifetime broadening, in agreement with experiment.

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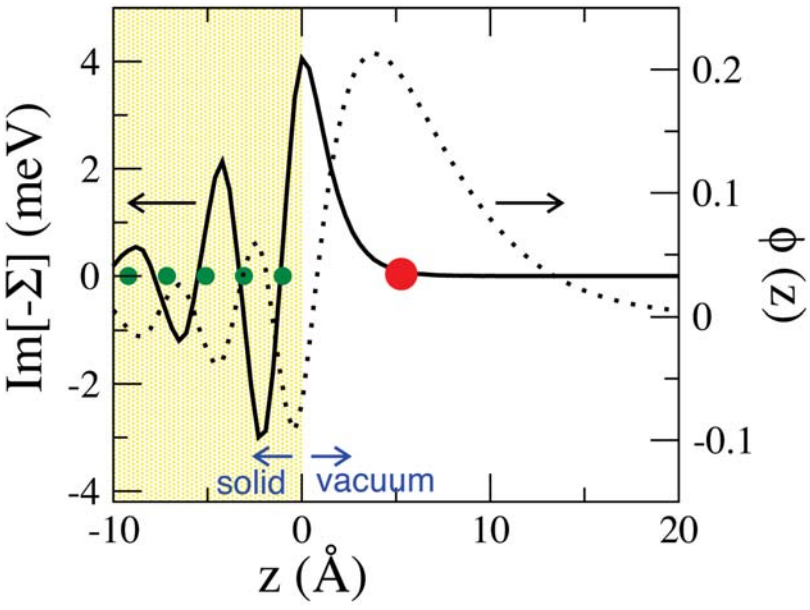

Wave function and imaginary part of the n=1 image state self-energy

DIPC Highlight

Nonlinear Screening in Two-Dimensional Electron Gases

by *E. Zaremba*[1,2], *I. Nagy*[3,2], *and P.M. Echenique*[4]

A charged impurity or projectile inmersed in a metal induces the rearrangement of the electrons around it, providing the total screening of the charge. Typically, the impurity represents such a strong perturbation that a nonlinear screening theory is needed to account for the modifications of the local electronic structure. The possible realization of quasi-two-dimensional systems in a variety of contexts (semiconductor heterostructures, electrons on the surface of liquid helium, layered materials...), has led us to study the screening of a point charge in a *two-dimensional* electron gas using a *density functional method*. In marked contrast to the three-dimensional case, we find that the screened potential for a proton supports a bound state even in the high-density limit.

In the high density limit, the screening density in a two-dimensional electron gas is simply proportional to the perturbing potential.

Today condensed matter physics is by far the largest field of physics. It is concerned with the study of solids. A subtle task considering the huge number of particles one has to deal with (a mollar quantity of a solid contains as many as 10^{23} atoms). Different theories have been developed in finding approximations to handle this problem. Among them, modern density-functional theory (DFT) makes two kinds of contribution to the science of multiparticle quantum systems. The first is in the area of fundamental *understanding*, since DFT focuses on quantities in the real coordinate space, principally on the electron density n(r). This quantity, similarly to the exchange-correlation hole density, is physical and transparent. Their understanding provides a complementary insight into the nature of multiparticle systems. The second contribution is *practical*. The theory leads to self-consistent field equations, similar to the Hartree equations, in which the effects due to the interparticle Coulomb interaction and the Pauli exclusion principle are included by addition of the exchange-correlation potential.

The capability of this practical mapping between the real, interacting many-electron system and an idealized system of noninteracting electrons moving in an effective single-particle potential, still remained as a nontrivial question for reduced dimensions. The possible realization of two-dimensional (2D) electron systems in a variety of context (semiconductor heterostructures, image or band-gap surface states at metal surfaces, and layered materials) confirms the relevance of this question. In all these cases, the interaction of external charges with the two-dimensional electron gas (2DEG) is a problem of both fundamental and practical interest. Experimentally, the powerful scanning tunneling microscopy offers a direct means of determining the modulated electron density through the observation of induced Friedel oscillations. Furthermore, transport of elec-

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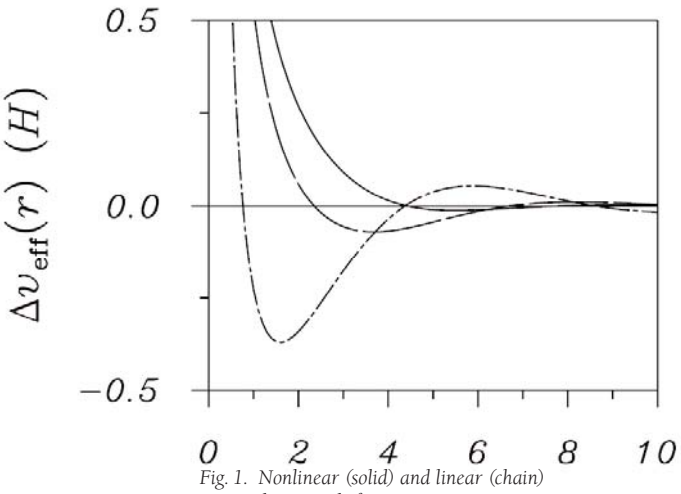

Fig. 1. Nonlinear (solid) and linear (chain) screened potentials for an antiproton

trons is often limited in real matter by impurity scattering and, thus, a detailed knowledge of the scattering potential is also needed. All these reasons motivated us to investigate within the context of DFT, the nonlinear screening of a point charge, Z, located in the plane of a 2DEG.

As is the case in 3D, the screening potential of a negatively charged impurity (an antiproton, for instance) repels electrons almost completely from the charge, leaving exposed the positive background of the metal, which neutralizes the impurity. This repulsion, however, is not enough to create an attractive potential sufficiently strong to bind an electron, as was suggested in a linear treatment of the screening.

The results for a positive impurity are quite different. In marked contrast to the situation in 3D, we find that the screened potential for a proton supports a bound state even in the high-density limit. This result would invalidate the applicability of perturbation theory in this limit. We prove, however, that the results of linear theory are in fact correct even though bound states exist. These results find application in a variety of problems, such as charged impurity scattering and the stopping power of charged projectiles, we also calculated. ■

In a two-dimensional electron gas, a proton can bind two electrons even in the high density limit.

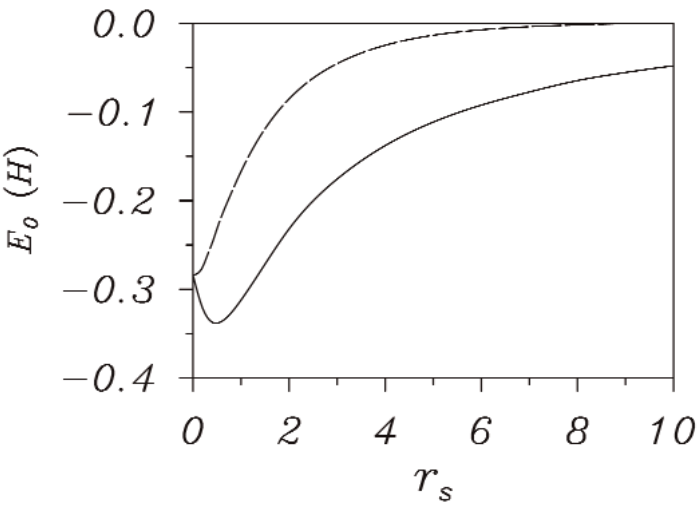

Fig. 2. Bound state eigenvalue for a proton as a function of the 2D electron gas density

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DIPC Highlight

Non-gaussian Nature of the α-relaxation of Glass-forming Systems*

by *J. Colmenero[1,2,3], A. Arbe[2], F. Alvarez[1,2], M. Monkenbusch[4], D. Richter[4], B. Farago[5] and B. Frick[5]*

Molecular dynamics (MD) simulations on glass forming systems of very different nature (Selenium, ortotherphenyl, water,...) have shown a series of "universal features" for the non-Gaussian parameter $\alpha_2(t)$ corresponding to the self-motion of the atoms in the α-relaxation regime. A combination of MD-simulations and neutron scattering on polyisoprene has allowed us to establish that the above mentioned "universal features" of $\alpha_2(t)$ can also be found in glass-forming polymers, and are nicely captured by a simple anomalous jump diffusion model with a distribution of jump lengths.

How do atoms move during the structural relaxation? Key to understand the glass transition!

One of the most intriguing problems in condensed matter physics is the glass transition phenomenon, caused by the freezing of the structural (α) relaxation in a glass-forming system. Therefore, the understanding of the molecular motions during this relaxation is of utmost importance to shed some light on the glass formation process. Neutron scattering (NS) and Molecular Dynamics (MD) simulations are essential for this goal. During last years, extensive NS investigations of the incoherent scattering function $F_s(Q,t)$ have established a universal behaviour for the self-atomic motions in the α-relaxation regime of glass forming systems including polymers. As Figure 1 evidences, $F_s(Q,t)$ shows a stretched exponential functional form characterized by the exponent β:

$$F_s(Q,t) \propto \exp[-(t/\tau_w)^{\beta}] \quad (1)$$

with a characteristic time τ_w that clearly depends on Q, $\tau_w(Q)$. This observation implies the diffusive nature of the atomic motions in this regime. Further-more, in the Q-regime approx. $0.2 \le Q \le 1.5$ Å^{-1} the Q-dependence of τ_w in polymers can be described as $\tau_w(Q) \propto Q^{-2/\beta}$ (inset of Fig. 1), implying a Gaussian form of $F_s(Q,t)$ with negligible values for the non-Gaussian parameter $\alpha_2(t)$.

This is in apparent contradiction to results from MD-simulations on glass forming systems other than polymers. There, $\alpha_2(t)$ shows a maximum that increases with decreasing temperature and shifts according to the thermal behaviour of the structural relaxation time. Thus the question arises: Do glass forming polymers behave in a different way? To answer this question we decided to take a twofold approach: we performed fully atom-

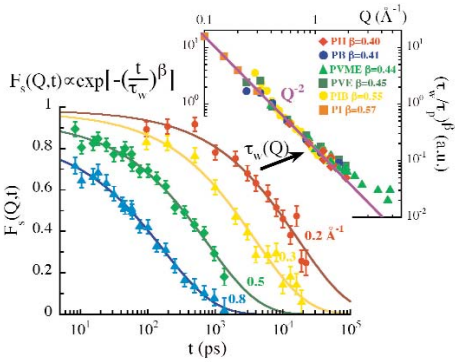

Figure 1: $F_s(Q,t)$ measured on PI at 340 K. Solid lines: fits with Eq. (1). Inset: master curve giving the Q-dependence of τ_w^{β} built with results from six different polymers (see legend), applying polymer-dependent normalising factors (t_p). Solid line: Gaussian behaviour.

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istic MD-simulations and NS measurements on the same polymer, polyisoprene (PI) [1]. Figure 2 shows the obtained Q-dependence of τ_w. An impressive agreement is found between both kinds of results, validating the MD-simulations. The data univocally confirm the Gaussian-like behaviour in the Q-range approx. $Q \leq 1$ Å^{-1}, while clear signatures of deviations become evident at higher Q-values.

Having established confidence on the realism of our MD-simulations, we can take advantage of them and compute magnitudes that are not easily experimentally accessible, like $\alpha_2(t)$ and the mean squared displacement $\langle r^2(t)\rangle$ of the main chain protons. They are shown in Fig. 3(a), while Fig. 3(b) displays the calculated $F_s(Q,t)$ for several Q-values. As reported for the other glass-forming systems, a main maximum is indeed found for $\alpha_2(t)$ at $t^* \approx 4$ps, just in the early stages of the decaging process identified with the α-relaxation. The shadowed area in Fig. 3 shows the region where $\alpha_2(t)$ takes significant values. For low Q-values this area only covers the initial part of the slow decay (α-regime) of $F_s(Q,t)$. However, as Q increases, the marked time range starts to cover almost completely the slow decay. This naturally explains the finding of the deviations from Gaussian behaviour of $F_s(Q,t)$ at high Q-values. What could be the origin of such deviations? The way the characteristic time departs from the Gaussian expectation (Fig. 2) strongly reminds us on the very well known manifestations of the discrete nature of diffusion in simple jump diffusion models. Basing on this similarity, we have proposed a model that considers a distribution of elementary jump lengths underlying the anomalous diffusion undergone by the atoms in the α-process [1]. Such an extremely simple approach allows a very accurate description of the Q-dependence of τ_w (Fig. 2). The associated distribution of jump lengths $f(\lambda)$ (inset of Fig. 2) shows a maximum at about 0.4 Å. This model also semiquantitatively reproduces the behaviour of $\alpha_2(t)$ [see Fig. 3(a)], within its range of validity (above 1 ps approximately) [1]. It is finally noteworthy that the main "universal features" reported in the literature for $\alpha_2(t)$ are also naturally deduced in this approach [1]. This suggests that the essence of the universal deviations from Gaussian behaviour in the self-motions of atoms during the structural relaxation regime lies in the distribution of discrete steplengths underlying the anomalous diffusion. ■

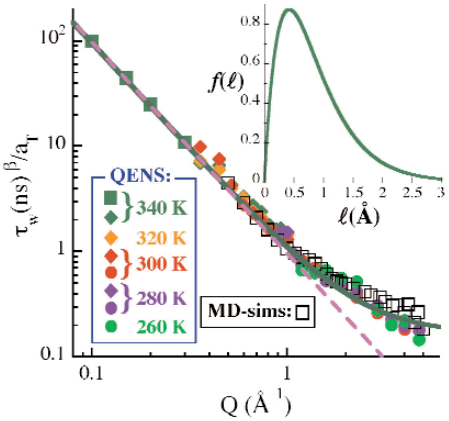

Figure 2: Master curve constructed combining NS and MD-simulations results for PI. T-dependent shift factors a_T have been applied. Dashed line: Gaussian prediction; solid line: description in terms of the anomalous jump diffusion model with the distribution of jump lengths shown in the inset.

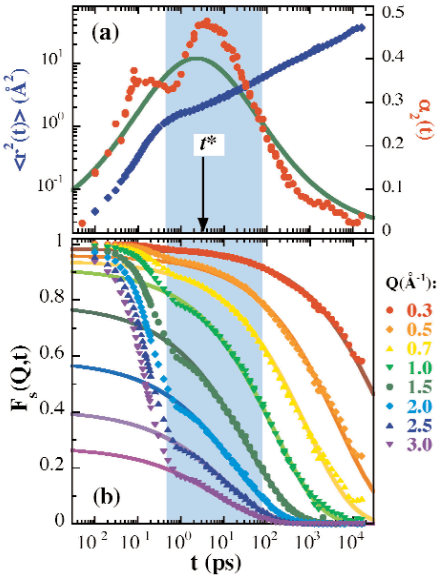

Figure 3: MD-simulations results for PI: (a) Time evolution of $\langle r^2(t)\rangle$ (◆) and $\alpha_2(t)$ (●). Solid line: anomalous jump diffusion model prediction for $\alpha_2(t)$. (b) Fs(Q,t). Solid lines: fits with Eq. (1) ($t \geq 5$ ps). The shadowed area covers the time range of the full-width at half-maximum of the main peak of α_2.

We find polymer behavior similar to other glass forming systems

Non-Gaussian behavior seems to reflect the discrete nature of the motions underlying the structural relaxation

*An extended version of this paper has also been recently published in the MODELLING section of the Scientific Highlights of the 2003 ANNUAL REPORT of the Institut Laue-Langevin (ILL), Grenoble (France)

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DIPC Highlight

Chain Connectivity and Segmental Dynamics of Miscible Polymer Blends

by *E. Leroy*[3], *A. Alegría1*,[2] *and J. Colmenero*[1,2,3]

We have experimentally demonstrated the ability of the effective concentration concept to quantitatively predict the component dynamics in three model miscible polymer blends.

Polymer blending is a convenient way for obtaining new materials with tailor made properties.

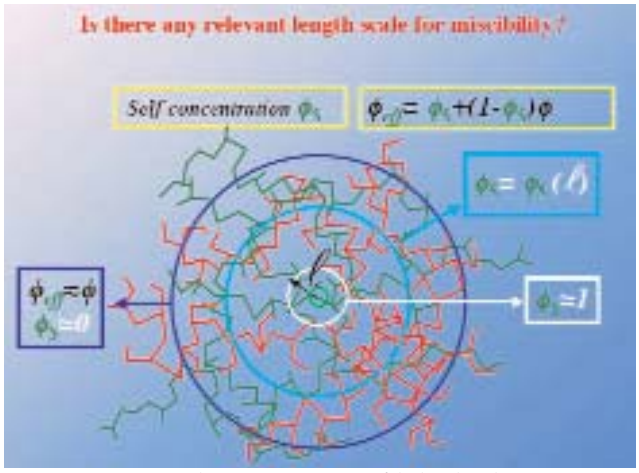

Figure 1: Schematic representation of the length scale dependence of the effective concentration.

Polymer materials, usually referred to as plastics, are found everywhere in the normal life. A route used to obtain new polymer materials is by combining already existing polymers, which allows tuning the desired properties of the resulting material. Among the broad range of multicomponent polymer materials, a family of both, fundamental and technological interest is that of the binary miscible polymer blends. These systems are homogeneous mixtures of macromolecular chains of two types. However, they present what is referred to as dynamical heterogeneity, i.e., the motions of the segments of the two polymer components occur with significantly different time scales. A way to understand the dynamic heterogeneity of miscible polymer blends is to consider the chain connectivity effects. In a miscible polymer blend A/B, the chain connectivity imposes that the local environment of a segment for instance of polymer A is (on average) necessarily richer in this component as compared to the bulk mean composition . Thus, the more flexible component of the blend will move faster than the more rigid one despite the system is miscible. To account quantitatively for this effect, the concept of effective local concentration has been introduced. The effective local concentration sensed by a polymer component, can formally be expressed as:

$$_{eff} = _{S} + (1 - _{S}) \quad \text{eq.1}$$

being $_{S}$ the so called "self-concentration" of the polymer segment considered. Obviously, the value of $_{eff}$ depends on the considered length scale, approaching unity for very short length scales and the average concentration, , for large length scales (see figure 1). Recently, it has been proposed that the relevant length scale for the polymer segmental dynamics (the molecular motions responsible of the glass transition phenomenon) is the Kuhn length (l_K), defined as the length along the chain contour that makes the orientation of a given chain bond to be independent of the orientation of the chain bond at the origin. On the basis of this assumption $_{S}$ can be calculated as the concentration of monomers of a given chain component within a volume $V \sim l_K^3$ centered in a segment of the same chain.

The existence of two different segmental dynamics in a miscible blend would imply the presence of two distinctive glass transition processes — and therefore they should

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depict two glass transition temperatures, T_g-each associated to one of the two polymer components. The way that has been proposed to calculate these effective glass transition temperatures $T_{geff}(\ )$ for each component in the blend is to use the concentration dependence of the macroscopic (average) glass transition temperature $T_g(\ )$, as measured in a standard differential scanning calorimetric (DSC) experiment, according to the following relationship:

$$T_{geff}(\ )=T_g(\ _{eff}) \quad \text{eq.2}$$

Dielectric measurements on miscible polymer blends can be used to investigate selectively a single component if the other does not contribute to the dielectric relaxation process. Taking advantage of this capability, in this work[1] we have tested in a quantitative way the accuracy of the effective concentration approach above described to account for the dynamical heterogeneity of miscible polymer blends.

Three model miscible blends have been studied by combining DSC and Thermally Stimulated Depolarization Current (TSDC). This second technique can be considered as a dielectric sensitive equivalent of DSC and it allows determining the glass transition temperature sensed by the dielectrically active segments present in the polymer blend. The three blend systems studied take profit of this selectivity. In poly(vinyl methyl ether)/polystyrene (PVME/PS), only the lower T_g component (PVME) is dielectrically active. In polystyrene/poly-o-chlorostyrene (PS/PoClS), PoClS is the dielectrically active and the highest T_g component. Finally, in PVME/PoClS both components are dielectrically active but with a very high T_g difference, which should allow to resolve the corresponding dielectric contributions. DSC measurements showed a single heat capacity step for all blends, confirming their miscibility. Some typical TSDC measurements are illustrated in figures 2. It is apparent that whereas for pure PVME both techniques provide essentially the same value of T_g, for the PVME/PS blends the TSDC peak maximum occurs at a temperature significantly different (lower) than the calorimetric T_g, (middle point of the heat capacity step). The glass transition temperatures obtained for the PVME/PoClS blends using both DSC and TSDC data are plotted on figure 3. To have a quantitative test of the "effective concentration" approach, for each

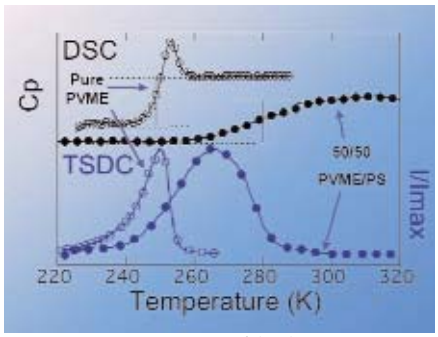

Figure 2: Determination of the glass transition temperatures. DSC: macroscopic T_g and TSDC: T_{geff} of the dielectrically active component.

Two different segmental dynamics would imply two distinctive glass transition temperatures.

blend system, we first fitted the concentration dependence of the bulk glass transition temperature measured by DSC. In a second step, we calculated the corresponding values of T_{geff} of the dielectrically active component according to eq 2. A remarkably good quantitative agreement between the experimental values and the calculated T_{geff} curves can be observed for all measured blends (see Fig. 3). This result demonstrates the ability of the effective concentration approach to account quantitatively for the dynamical heterogeneity of miscible polymer blends. Furthermore, this good agreement pointed out to l_k as the relevant length scale for the glass transition phenomenon in polymers, i.e. a few nanometers, which is much shorter than that commonly assumed. ■

Dielectric techniques allow us to investigate selectively the dynamics of a single component in blend systems.

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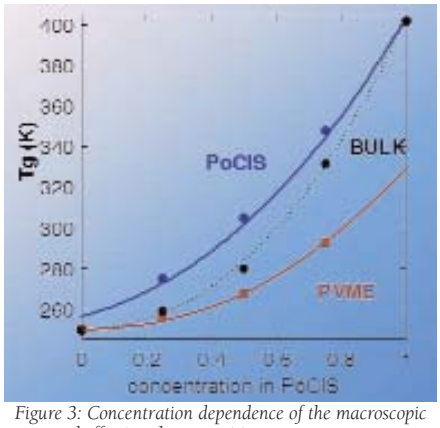

Figure 3: Concentration dependence of the macroscopic and effective glass transition temperatures on PVME/PoClS blends. The lines for the effective glass transition temperatures of the two components (solid lines) were obtained from that of the macroscopic $T_g(\ )$ (dotted line) using eq. 2.

The effective concentration concept captures quantitatively the dynamical heterogeneity of miscible polymer blends.

DIPC Highlight

Crossover from α-relaxation to Rouse Dynamics

by *A. Arbe1, J. Colmenero[1,2,3], D. Richter[4], M. Monkenbusch[4], L. Willner[4], B. Farago[5]*

We report on a large experimental effort exploring the dynamics of poly(vinyl ethylene) on length scales covering Rouse dynamics and below. The results establish for the first time the simultaneous existence of a generic sublinear diffusion regime which underlies the α-process in addition to the Rouse process. Both regimes are separated by a well defined dynamic cross over. From that the size of the Gaussian blobs making up the Rouse model is determined directly. The glassy dynamics is identified as subdiffusive motions occurring within these Gaussian blobs.

Is it possible to experimentally clarify the independent existence of a generic dynamic regime of sublinear diffusion associated with the α-process aside the Rouse process?

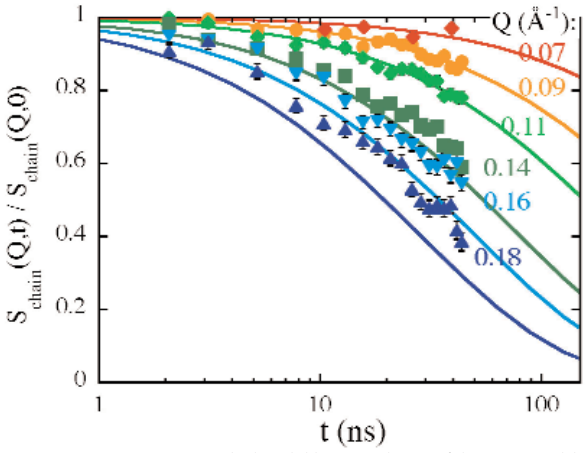

Figure 1. $S_{chain}(Q,t)$. Solid lines: prediction of the Rouse model.

Neutron Spin Echo gives the answer: It is!

Polymers show at the same time the general properties of glass forming systems — with the α-relaxation as the most relevant dynamical process —and features arising from their chain-like nature— the chain motions are described by the Rouse model, that treats the dynamics of a Gaussian chain (beads and springs) in a heat bath.

For a large number of polymers, neutron scattering studies performed at time scales close to the structural relaxation time t_s and in the Q-range 0.2 Å^{-1} ≤ Q approx. have shown that the protons perform sublinear diffusion with a mean-square displacement (msd) $\langle r^2(t)\rangle \sim t^{\beta}$ (β: stretching exponent, $0.4 \leq \beta \leq 0.6$) [1]. This behavior is similar to that predicted by the Rouse model ($\langle r^2(t)\rangle \sim t^{0.5}$). On the other hand, molecular dynamics (MD) simulations [2] and Mode Coupling Theory (MCT) calculations [3] on coarse-grained polymer models (bead and spring models) show the existence of a subdiffusive regime ($\langle r^2(t)\rangle \sim t^{x}$, $x \approx 0.5$-0.6) after the plateau reflecting the "cage effect". This regime was related to the Rouse dynamics of polymer chains. Furthermore, also quasielastic neutron scattering experiments on glass forming polymers taken at high Q were interpreted in terms of Rouse motion [4]. However, in real polymers the precondition of Gaussian beads can only be fulfilled on larger scales. The question thus arises: is it possible to experimentally clarify the independent existence of a generic dynamic regime of sublinear diffusion associated with the α-process aside the Rouse process?

We have performed Neutron Spin Echo (NSE) measurements on the single chain dynamic structure factor $S_{chain}(Q,t)$, related to the collective segment motion within one chain, and the self correlation function $S_{self}(Q,t)$, originated from the proton self motion, for poly(vinyl ethylene) (PVE). The

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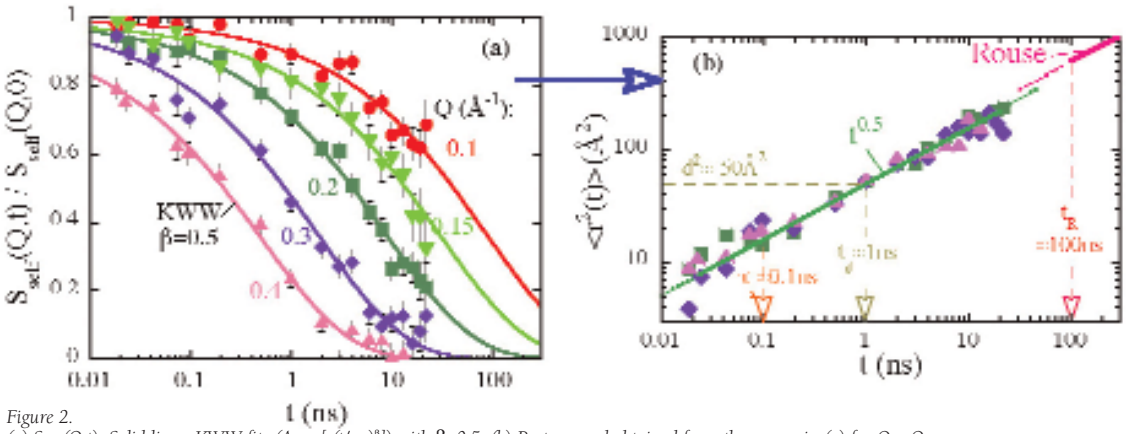

Figure 2.
(a) $S_{self}(Q,t)$. Solid lines: KWW fits ($Aexp[-(t/\tau_w)^\beta]$) with β=0.5. (b) Protons msd obtained from the curves in (a) for $Q > Q_R$.

instruments used were IN15 (ILL) and the NSE spectrometer at the FRJ-2 (Jülich). For a first time we have been able to distinguish clearly two separated dynamic regimes of sublinear diffusion [5].

Figure 1 compares the experimental $S_{chain}(Q,t)$ with the Rouse prediction. For small Q the data follow well the theory. Thus, in this Q-range the particles within the chain perform sublinear diffusion: $\langle r^2(t)\rangle \sim t^{0.5}$. However, at the highest Q's investigated ($Q > Q_R = 0.11$ Å^{-1}) severe deviations are evident (see the figure).

Turning to $S_{self}(Q,t)$ (Figure 2(a)), we can proof the existence of a second Gaussian subdiffusive regime at short length scales by the construction of a Q-independent msd [Figure 2(b)] for $Q \geq 0.20$ Å^{-1}. This follows $\langle r^2(t)\rangle \propto t^{0.5}$ (solid line). Thus, for $t < t_R = \tau_w^{Rouse}(Q_R) \approx 100$ ns the data reveal a subdiffusive regime which is obviously distinct from the Rouse process. This regime is indeed that relevant for the α-relaxation: both, τ_s as well as the time a proton moves as far as the average intermolecular distance d, lie in this region (see the figure) [5]. For $t \geq t_R$, the mean squared displacements follows the Rouse prediction $\langle r^2(t)\rangle^{Rouse}$.

The cross over between the Rouse- and the subdiffusive α-regime becomes most clear if we focus on the Q-dependent characteristic relaxation times (Figure 3). The two regimes are separated by a step at $Q_c \approx 0.13$ Å^{-1}. A cross over length scale $l_c \approx \pi/Q_c = 24$ Å may be obtained, that would be identified with the size of a Gaussian blob underlying the Rouse model. For PVE this corresponds to about ten monomers or twenty bonds. The α-process evolves then from the motion of the atoms within the polymer which are subject to specific intra- and inter-molecular forces. The coarse grained MD-simulations and MCT calculations based on bead and spring models [2,3] do not reveal this α-regime, since it appears to relate to the internal dynamics within the Gaussian blobs. ■

A cross over length scale lc ≈ 24 Å (≈ ten monomers) defines the size of a Gaussian blob underlying the Rouse motion. The α-process relates to the internal dynamics within the blobs.

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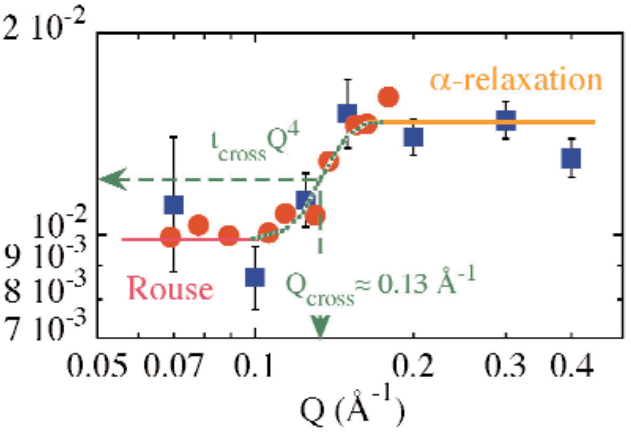

Figure 3. $\tau_w Q^4$ from $S_{self}(Q,t)$ (full squares) and deduced from $S_{chain}(Q,t)$.

DIPC Highlight

Rings Dancing in The Disorder*

by *S. Arrese-Igor[1], A. Arbe[2], J. Colmenero[1,2,3], A. Alegría[1,2] and B. Frick[4]*

By means of quasielastic neutron scattering we have studied the phenylene rings' dynamics in the engineering thermoplastic polysulfone in the glassy state. The wide dynamic range covered has allowed us to identify the simultaneous occurrence of fast oscillations and π-flips. A model combining these two motions nicely describes the results in the whole dynamic range investigated. The structural disorder characteristic of the amorphous state leads to broad distributions of characteristic times.

Understanding the molecular motions underlying secondary relaxations in polymers can help to design materials with tailor made properties.

Have you ever realized the importance of plastics in your daily life? Look around. You can find them in your computer, printer, furniture, car,...everywhere. This is because they are durable, light, cheap, and their good mechanical and thermal properties make them suitable for a huge number of applications. Engineering thermoplastics like polycarbonate or polysulfone have for these reasons a salient important technological significance. Their interesting ultimate mechanical properties are probably related to the ability of these polymers to accommodate a stress with highly activated molecular motions, in these cases likely involving π-flips of their phenylene rings. That is why considerable efforts have been made to identify the molecular origin of the so called secondary relaxations in polymers. Though the existence of these processes and their main general features are established for many decades, their microscopic origin remains elusive. This is due to the fact that they have traditionally been studied by relaxation techniques like Mechanic (MS) and Dielectric (DS) Spectroscopy that do not provide microscopic information and space resolution. On the other hand, the few existing Neutron Scattering (NS) studies on the molecular motions behind the secondary relaxations in polymers have been performed close or above the glass transition temperature T_g, where the main α-relaxation is also active.

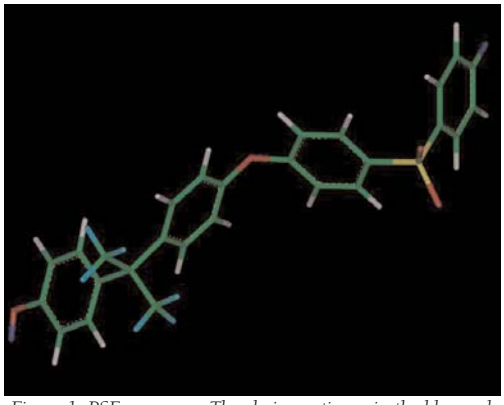

Figure 1. PSF monomer. The chain continues in the blue ends.

Here we have exploited NS capabilities for deciphering the microscopic motions undergone by polysulfone phenylene rings deep in the glassy state with a twofold aim: contribute to the fundamental question about the origin of secondary relaxations in polymers and provide useful information for further design of plastics with tailor made mechanical properties.

The measurements were performed at the Institute Laue-Langevin (ILL) on polysulfone (T_g = 460 K) with deuterated methyl groups (Figure 1), covering the micro- (≈ 0.1 ps to 20 ps) and mesoscopic (≈ 100 ps to 1 ns) timescales. The spatial resolution of NS techniques has been exploited to identify the nature of the dynamical processes detected. The geometry of the motions involving

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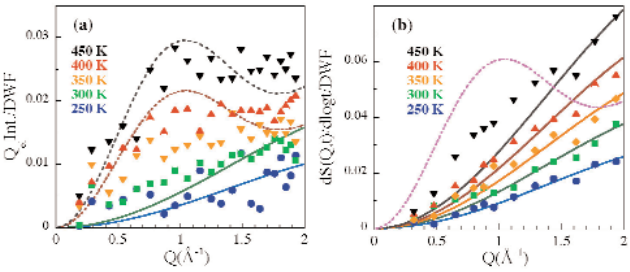

Figure 2: Q-dependence of the magnitudes reflecting the geometry of the motion in the mesoscopic (a) and microscopic (b) timescales. Lines indicate the expectation for jumps of the aromatic protons between two equivalent positions separated a distance d= 4.3 Å (dashed lines) and d= 1.5 Å (solid lines).

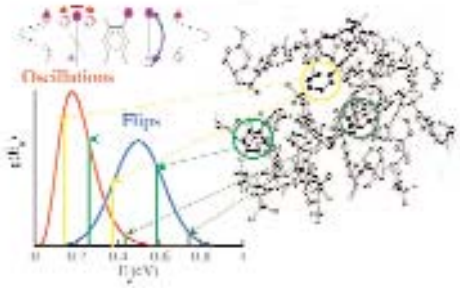

Figure 3: Activation energy distributions for the flip and oscillatory motion.

phenylene rings can be envisaged through the Q-dependence of the scattered intensities. As commented above, a movement that is suspected to occur is a π-flip of the phenylene ring. Then the motion of the aromatic hydrogens would correspond to a jump over two equivalent positions separated by 4.3 Å, leading to a maximum in the quasielastic intensity at about 1 $Å^{-1}$. Is this expectation realized in our experiments? Look at Figure 2. For the highest temperatures investigated, the motion observed in the mesoscopic window indeed corresponds to such a flip. However, on the other extreme, the lowest temperatures showing relaxational features on the microscopic window display a completely different Q-modulation, that would reflect a much more restricted motion in space (amplitudes of ≈ 1.5 Å). This dynamical process might be interpreted as phenylene ring small angle oscillations around the main chain axis, and clearly dominates in the microscopic window. However, with increasing temperature contributions of the π-flips also appear there (see the clear "bump" at 450 K). In a similar way, at mesoscopic scales the high Q-intensity resolved at T ≤ 300 K indicates the contribution of the small amplitude motions. Thus, both processes contribute to both windows. A global description considering the two motions is necessary to reproduce the experimental results in the full dynamic range investigated.

A model considering statistically independent π-flips and small angle oscillations for phenylene ring motion [1] allows a nice description of the experimental observations. Reflecting the effect of disorder in these relaxation mechanisms, broad distributions of activations energies have to be invoked (Figure 3). They are originated by the packing heterogeneity characteristic for the amorphous nature of polymers. The mean activation energy value obtained for the flips, ≈ 0.43 eV, agrees well with that found by spectroscopic techniques in similar systems for the secondary γ-relaxation—responsible for the good mechanical properties. On the other hand, the oscillations show an amplitude that increases with temperature and a mean activation energy, about 0.2 eV, close to that determined for methyl group rotations by NMR and the δ-relaxation by MS. In the proposed scenario, the apparent activation energy for flips would represent a real potential barrier over which the phenylene ring jumps. In contrast, oscillations would take place – probably correlated with other fast motions with small associated spatial scales like methyl group rotations — as a result of rapid fluctuations of the single particle potential seen by the phenylene ring, and produced by the surrounding atoms. In this case, the apparent activation energy for oscillations would only reflect the characteristic time of such fluctuations.■

Neutron scattering allows to identify two kinds of motion for phenylene rings

Disorder leads to broad distributions of barriers

The microscopic motions here unveiled seem to be responsible for the secondary relaxations observed by spectroscopic techniques

*An extended version of this paper has also been recently published in the SOFT MATTER section of the Scientific Highlights of the 2003 ANNUAL REPORT of the Institut Laue-Langevin (ILL), Grenoble (France)

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OUR RESEARCHERS

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

Index

Fellows Gipuzkoa*

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. 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. R. Díez Muiño

Lawrence Berkeley National Laboratory, Berkeley, California, USA

01-12-2000 through 02-03-2003

· Photoemission and photoelectron diffraction at surfaces. Photoelectron spectra of gas-phase molecules.

· Ion-solid interactions: electronic excitations and charge-transfer processes.

· Electron excitation spectrum of non-periodic systems: response function of impurities, metallic clusters.

Dr. V. Silkine

Russian Academy of Science, Tomsk, Russia

03-01-2002

The theoretical investigations of dynamics of quasiparticles in the surface and image potential states for clean Pd and Al metal surfaces as well the Cu(100) and Cu(111) surfaces covered by alkali atoms with the use of model potential and first principles pseudopotential approaches have been performed. For the alkali/Cu(100) and alkali/Cu(111) systems the importance of L and X band gaps of bulk Cu for the relatively long lifetime of the excited alkali induced transient states is shown. On base of model potential calculation of surface dynamic screening, it has been demonstrated the possibility of formation of a novel low-energy collective electronic excitations at the metal surfaces with partly occupied s-p_z surface electronic band.

**program supported by Provincial Authority of Gipuzkoa*

Post-doctoral Positions

Dr. A. Ayuela

*Member of Etortek**
Universidad de Salamanca, Spain
14-01-2002

· 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.
· Studies of new materials: Nanotube functionalization and cement.

Dr. L. Blanco

Universidad de Salamanca, Spain
14-01-2002

The effect of nanoparticles in the spontaneous emission from a nearby atom is studied by calculating the emission probability and the distribution of the far and near field for various nanoparticle shapes and atom positions. In particular, strong concentrations of the electromagnetic field both in the proximities of a point near the source and in a definite direction at large distances can be achieved when the geometry is appropriate. The obtained results can be used in several applications for microwave antennae.

Dr. M. Grüning

Universiteit van Amsterdam, Holland
15-11-2003

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. R. Keyling

Fritz-Haber-Institut, Berlin, Germany
15-10-2002

Caused by several photoemission experiments my work at DIPC is focused mainly on the electron-electron and electron-hole interaction and the appropriated self energy.
The work is split in two parts:
1. ground states; performance of ab-initio calculations in the framework of DFT, using LDA, GGA, TDLDA
2. excited states; many-body perturbation theory, GW-calculations of quasi-particle properties like quasi-particle band structures and lifetimes.
All these will be applied to various bulk and surface systems, especially metals, transition metals and alloys.

Dr. E. Leroy

UMR CNRS, Lyon, France
01-05-2001 through 30-09-2002

Study and modelization of the component segmental dynamics in miscible polymer blends using dielectric spectroscopy, particularly in the case where only one component of the blend is dielectrically active, this component being either the one having the lower glass transition temperature (PVME in PVME/PS blends) or the higher one (PoCIS in PS/PoCIS blends).

**Etortek is a project supported by the Basque Government along with other technology centers.*

Dr. C. Lorthioir

Université Paris Sud, France

01-10-2001 through 30-09-2003

Local dynamics in miscible polymers blends: a dielectric relaxation and a neutron scattering study.

Confining polymer chains within geometries of nanoscopic dimensions induces deep changes in their static and dynamic properties. The investigation of confinement effects is a challenging question of fundamental interest. In the current work, we are studying two kinds of polymeric systems where self-confinement effects occur: the first is characterized by an ill-defined confining structure whereas in the other, the confining distance is very well-defined.

The first type of investigated systems is the homogeneous phase formed by miscible blends of polystyrene (PS) and poly(vinyl methyl ether) (PVME). We have mainly considered the high PS weight fraction regime (PS amount higher than 50 wt %). Even though a single glass-transition temperature Tg is observed by DSC in these PS/PVME blends, the two components exhibit a strong difference in mobility, at the segmental level. Thus, close to Tg, the PS/PVME blends offer a good avenue to study fluid (PVME) chains three-dimensionally confined in a glassy (PS) matrix. The dynamics of the PVME segments is selectively probed by broad band dielectric relaxation spectroscopy (10-3 - 10+7 Hz). On the other hand, neutron scattering techniques are used to characterise the structural properties of the confined systems (intermolecular structure of PS within the blends).

The second kind of studied systems are block copolymers. Ordered nanostructures exhibited by block copolymers allow studying the dynamics of polymer chains restricted in various confining geometries. The present work is focused on 1D-confinement displayed by lamellar phases of poly (dimethylsiloxane) (PDMS) and poly(styrene) (PS) block copolymers: PS-PDMS diblocks and PS-PDMS-PS symmetric triblocks of twice molecular weight. The strong incompatibility between PS and PDMS ensures thin interfacial regions and thus, a well defined confining distance. The dynamics of the "fluid" PDMS chains confined between the glassy PS blocks was probed at two different spatial scales, using NMR and broadband dielectric relaxation spectroscopy.

Dr. J. Sacristán

ICTP-CSIC, Madrid, Spain

01-04-2002

The focus of our research is on the simulation of materials properties of macromolecular (polymer) systems.

Through polymer computer simulations it is possible to gain insight into physical phenomena where the accuracy and scope of experimental results is limited. It is also useful to get a better understanding of their behaviour and their macroscopic properties with the help of atomistically detailed models.

The study of the structure of polymer surfaces and thin polymeric films at the atomistic scale is of interest for application and basic research.

We are interested in the following topics:

· Dynamics of amorphous polymer thin films between walls.

· Polymer dynamics from the local to the mesoscopic scale.

Dr. F. Schiller

Universität Dresden, Germany

01-10-2003

Quasiparticle lifetimes in low dimensional systems and nanostructures

A large variety of low dimensional systems and nanostructures, such as thin films, arrays of quantum dots and wires, or atom and molecule chains can be tailored by growing on solid surfaces with precise, atomic-level control. Due to reduction of dimensions such systems exhibit exotic electronic properties, like quantized states, charge density waves or strong correlation. In many cases the density of electron states at the Fermi energy can be modulated by size-dependent shift of quantum levels. This can affect transport and structural properties (e.g., Peierls distortions), as well as many-body effects. In particular the lifetime of hole or electron excitations depends on the availability of electron states at the Fermi energy. In this project we want to investigate by means of High Resolution Photoemission quasiparticle lifetimes in a number of low dimensional structures, which will be grown and analyzed by Scanning Tunneling Microscopy in San Sebastian.

Temporary Contract Positions

Dr. V. Joukov

Institute of Solid State Chemistry, Ural Branch of Russian Academy of Sciences, Ekaterunbourg, Russia

25-09-1999

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. Skliadneva

Institute of Strength, Russian Academy of Science, Tomsk, Russia

24-04-2003

"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

J. Cordón
Universidad de Cantabria, Spain
01-08-2002 through 31-10-2002
Ag/Co stripes and one-dimensional nanostructures.

A. Eiguren
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-11-2002 through 30-11-2003
The study of quasiparticle lifetime is of paramount importance for the understanding of the dynamical processes at metal surfaces. Electron-electron and electron-phonon interaction constitute the most important scattering channels of electronic states at clean surfaces.
We have focused our attention on the electron-phonon interaction at metal surfaces. In particular we have studied the following systems:
· Cu(111), Ag(111), Al(100) and Au(111) surface states.
· Cu(100) and Ag(100) n=1 image states.
· Be(0001) surface state.

I. García de Gurtubay
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-10-2003
Dynamical electron density response and many body effects in solids.

A. García Lekue
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-11-2002 through 31-03-2003
Theoretical investigation of many-body electronic properties on metal surfaces:
· Dynamical response of metal surfaces to external perturbations; electronic scattering and energy-loss processes.
· Inelastic relaxation processes of low-energy electrons in metals: bulk and surface states. Influence of occupied d-bands on the decay of excited electrons and holes in noble metals.

A. Leonardo
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-09-2003
Electron-phonon interaction and electron (hole) lifetimes in quantum-well states in overlayers on metal surfaces.
Recent photoemission experiments showed very strong dependence of electron-phonon interaction in overlayer quantum-well states (QWS) on number of deposited layers on metal substrates. This can affect very much electron (hole) dynamics in QWS. In the present project first-principle calculations of electronic structure, vibrational modes, electron-phonon coupling parameter and the phonon contribution to the electron (hole) lifetimes are performed for overlayers on beryllium, copper, and silver substrates. It is shown that all these quantities are radically modified compared to bulk materials. For instance, electron-phonon couping parameter can be changed by 200-400%.

M. Machado

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-11-2002 through 30-06-2003

Several problems related with electron dynamics at metal surfaces are being treated:
· Importance of screening in the decay processes of surface state electrons and holes.
· Lifetimes of image states at metal surfaces with dielectric overlayers.
· Electron-hole pair creation processes by scattering of noble gas atoms on metal surfaces. Influence of response function and surface state.

A. Mugarza

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01-11-2002 through 28-02-2003

Measuring electron wave functions of lateral nanostructures by means of photoemission. Angle-resolved photoemission is unique to thoroughly probe electron wave functions in reciprocal space. Since the probability density is the physical observable, direct Fourier transformation to real space is lacking phase information. However, in nanostructures grown on a surface, such as dots, wires or stripes, the wave functions are confined laterally and hence phase retrieval iterative procedures can be applied. In fact, using electron surface states confined to terraces on stepped surfaces, we have shown that is possible to recover electron wave functions in real space directly from photoemission data, applying the oversampling method of x-ray diffraction.

R. Pérez

Universidad de Valladolid, Spain
15-11-2003

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.

M. Quijada

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
15-09-2003 through 31-12-2003

ELECTRON DYNAMICS IN METAL CLUSTERS

The study of electronic excitations and of electron dynamics is one of the keys to determine the reactivity of metal clusters, either isolated or adsorbed on different kinds of surfaces. Our purpose in this project is the theoretical study of some excited-state electronic properties of metal clusters, and more precisely, the analysis of the size-dependent effects that arise in the lifetimes of electronic excitations at metal clusters. In a simplified picture, electrons excited in a metal cluster keep their energy for a given period of time (called lifetime) until they decay into a quantum state of lower energy. From the experimental point of view, time-resolved femtosecond techniques are powerful tools to study ultrashort electron dynamics in metallic systems in real time [1,2]. However, a detailed theoretical analysis of such processes is still missing, although it is essential to understand the basic mechanisms of cluster reactivity.

S. Riikonen

University of Helsinki, Finland

01-02-2003 through 31-03-2003

The work is centred in the theoretical study of the Si(111)-(5x2)-Au and other related surface reconstructions originated in silicon surfaces after the deposition of gold and other noble metals. The 5x2 reconstruction is characteristic of relatively flat (i.e. close to the (111) orientation). It has been extensively studied with different experimental techniques and there are plausible structural models. However, before 2003, there were no theoretical studies of this surface. Starting from the experimentally proposed models we have refined them using first-principles molecular dynamics, and study the electronic properties of our equilibrium configurations. We have found at least two possible candidates for the surface structure with competing stabilities. One of the models is basically identical to that proposed very recently by S. C. Erwin, while the other one represents a completely new structure. The main difference between these structures arises from the different location of the surface dislocation characteristic of the 5x2 reconstruction. Our data on the electronic structure has been compared with recent photoemission data, where a puzzling continuous transition from two to one-dimensional character in the states of the most prominent electronic band was found. Both structures give a reasonable agreement with these data, although the agreement seems to be somewhat better for the newly proposed structure. The STM images of both surface models have been simulated being also in good agreement with the experimental information.

I. Romero Perez

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01-12-2003

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 sustain electric and magnetic resonances over a wide range of wavelengths.

A. Rodriguez Prieto

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain.
01-08-2003 through 30-09-2003
Pressure induced complexity in a lithium monolayer.
The light alkali metals have usually been considered as simple metals due to their monovalency and high conductivity. The nearly free electron model (NFE) is quite accurate for these systems at normal conditions, because the pseudopotential is weak as a consequence of the repulsion that valence electrons experience, related to the Pauli exclusion effects by the core electrons. However, recent results have proved that, at high pressure, their behavior deviates radically from a NFE model, due to the growing pseudopotential with increasing density. We perform ab-initio calculations to analyze the deviation from simplicity induced in a lithium monolayer when pressure is applied. The surprising "Tight-Binding" type nesting observed in the Fermi surface of the monolayers a result of the increasing non-local character of the atomic pseudopotential induces an interesting correlation of its structural, electronic and even magnetic properties, which are analyzed in order to understand the physical origin of the observed complexity.

M. Ruiz Oses

Universidad de Cantabria, Spain
05-05-2003 through 30-06-2003 and 01-09-2003 through 31-10-2003
Experimental surface science, focused on the morphology and the electronic states in nanostructures. We use two experimental techniques: Scanning Tunneling Microscopy (STM) and Angle-resolved Photoemission, with synchrotron radiation.

R. Vincent

Université de 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.

[1] R. Pfandzelter, T. Bernhard, and H. Winter, Physical Review Letters **86**, 4152 (2001).

VISITING RESEARCHERS

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

Index

Long Visits

Prof. J. Alonso

Universidad de Valladolid, Spain
01-09-2002 through 31-08-2003

During my Sabatical stay at DIPC, I have investigated on several topics in the general field of Nanostructures, in collaboration with DIPC and UPV scientists and students.

· Structural and chemical properties of carbon nanotubes: Absorption and storage of Hydrogen. Intercalation of alkali atoms in graphite and nanotubes. Computer simulation of the formation process and growth of nanocones.

· Electronic and chemical properties of atomic clusters: Optical properties. Interaction of metallic clusters with Hydrogen. Metastable states of multiply charged clusters. The dynamics of excited states in density functional theory, with applications to molecular dissociation and Coulomb explosion in nanostructures.

· Electronic correlations in atoms and clusters.

Dr. F. Auzel

CNRS, UMR, Meudon, France
28-10-2003 through 30-01-2004

Powder coherent sources both of the superradiant (SR) and Amplified Spontaneous Emission (ASE) types [1,2,3,4].

Dr. A. Borisov

Université Paris Sud, France
01-05 through 26-06-2003

"Building up the screening below the femtosecond scale"

Time dependent density functional theory is used to study short-time dynamics of the screening of charges suddenly introduced in a free electron gas. The electron gas is modeled with a finite-size jellium cluster. We find that the screening is built-up locally on a time scale well below the femtosecond for typical metallic densities. At this ultrashort time scale, the time evolution is not affected by the cluster boundary conditions, and our results apply to the infinite system as well. The results for different electronic densities can be understood in terms of universal scaling laws.

Prof. A. Galindo

Universidad Complutense Madrid, Spain
09-11 through 20-12-2003

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. B. Gumhalter

University of Zagreb, Croatia
01-11-2001 through 28-02-2002
Several topics have been planned to be studied and discussed with the researchers and Ph.D. students during the visit to the DIPC:
· Decoherence effects associated with spatio-temporal propagation of electron-hole pairs optically excited in the bands of image potential at metal surfaces.
· Asseessment of the respective roles of plasmons and electron-hole pairs in two-dimensional surface bands in the screening properties of surfaces.
· Effects of electron-hole copuling on the lifetime of quasiparticles in the states of surface potential.
· Excitation of surface phonons or charge density fluctuations in scattering of atoms and molecules from metal surfaces.

Dr. W.A. Hofer

University College London, U.K.
14-09 through 31-10-2002
First Principles Calculations of Electronic Structure of Solid Surfaces using the DFT code VASP, as well as obtaining STM images using his own code bSKAN. Since then, he is collaborating with Andres Arnau in a project to study inelastic tunneling currents in metallic contacts and another one to characterize the adsorption of Oxigen on Ruthenium (0001) surfaces.

Prof. A. Kaminskii

Russian Academy of Sciences, Russia
02-10 through 31-12-2002
Professor Alexander A. Kaminskii is acknowledged leader in the basis research of the physics and spectroscopy insulating laser and nonlinear-laser crystals among the world solid-sate laser community. He is being recognized for his fundamental contributions in Ln3+-doped crystals and characterization of their spectroscopic and physical properties. Present scientific interests are in the field of nonlinear-laser crystals and nanocrystalline ceramics.

Dr. A. Kazanskiy

University of St. Petersburg, Russia
01-10 through 30-11-2003
Electron dynamics at adsorbates on metals

Dr. Y. Koroteev

Institute of Strenght Physics and Materials Sciences, Tomsk, Russia
01-12-2001 through 28-02-2002, 06-07 through 06-10-2002 and
26-02 through 26-05-2003
First-principles calculations of the surface electronic structure of La(001) and Lu(0001). First-principles film linear augmented plane wave calculations have been performed for La(0001) and Lu(0001). The d-surface states have been obtained at all symmetry points of the Brillanin zone. The dispersion of surface state at the _ point was used for interpretation of the scanning-tunneling spectroscopy measurements of the lifetime broadening on both Lu(001) and La(0001).

Dr. C. Lemell

University of Technology, Vienna, Austria
07-01 through 11-02-2003
Many Electron Systems Interacting with Strong Field.

Dr. M. Löffler

Lehrstuhl für Festkörperphysik, Erlangen, Germany
02-04 through 30-09-2002
Co and Ag nanostructures on Si surfaces.
Vicinal surfaces with high density of steps are natural templates for the growth of regular arrays of dots, wires and stripes. In this project we have studied by means of Scanning Tunneling Microscopy the reactive deposition epitaxy of cobalt silicides on vicinal Si(111) substrates. Contrary to initial expectations, the growth process is simplified with respect to the flat surface. A single precursor species, i.e. the Co ring structure, leads to a rapid buil up of silicide clusters, regularly spaced along the steps, although incoherently arranged across the terraces. Currently we are analyzing more quantitatively the different morphologies and stoichiometries observed as a function of coverage and deposition temperature.

Dr. J. Mahecha

Universidad de Antioquia, Medellin, Colombia
12-08 through 09-12-2002
Electron dynamics of atoms adsorpted in metallic surfaces
· Semi-classical propagation and spectral analysis in the negative Hydrogen ion interacting with a metallic surface: A semiclassical propagator method combined with harmonic inversion of short time signals is used to find the resonant states of an electron interacting with a H atom near a metallic surface. A semi classical propagator approach is used to calculate an approximation to the autocorrelation function entirely in terms of classical trajectories. A filter-diagonalization method for harmonic inversion of the complex time signal is applied to extract the resonances.
· Stabilization and complex scaling approaches to find resonant states of an electron interacting with an atomic core and a metallic surface are applied with similar purposes of those of (i) and using different models for the electron-surface interaction.
· The electron-core-surface system in the regime of large atom-surface distances is studied by using different methods. Initially a generalized van der Waals interaction model is used.
Tasks (i) and (ii) are developed with participation of two researchers of DIPC and (iii) with participation of two researchers of La Rioja University. Two students and a researcher from UdeA are involved in the development of the project.

Prof. I. Nagy

Technical University Budapest, Hungary
03-09 through 26-10-2002, 05-05 through27-06-2003 and
02-10 through 30-11-2003
Study based on a scattering approach of short-range correlations in an electron gas has been developed. In this work, the pair-correlation function at zero interparticle separation g(0) of an interacting electron gas is derived by an averaging procedure using the exact enhancement factor for scattered waves of electrons in a model potential. The range of

the screened potential is fixed by a physically motivated constraint. Agreement with the result of a many-body method based on summation of ladder diagrams for electron-electron interactions is established. As a possible application of the potential a nontrivial density-scaling in the thermal resistivity of metals is predicted.

Dr. V. Popov

Altai State Technical University, Barnaul, Russia
18-05 through 14-08-2002 and 01-12-2002 through 28-02-2003
Theory of excitations in small atom clusters.
Graund states properties of small magnetic clusters of 3d-atoms.

Dr. G. Roussina

Russian Academy of Sciences, Tomsk, Russia
03-04 through 14-06-2003
Surface phonons in CuPd surface alloyes.

Prof. W. Schattke

Universität Kiel, Germany
26-10 through 12-2002 and 01-12-2003 - 29-02-2004
Photoemission from core and valence levels in gas-phase atoms, solids and surfaces: We have developed a generalization of the multiple scattering theory to treat non-spherical potentials. This allows us to make a more accurate description of the photoemission process, which is relevant for many new experiments. For example, during the past few years the experimental advances have permitted the measurement of the angular distributions of photoelectrons emitted from free molecules fixed in space. Previous to this work, free-molecule studies were limited to orientationally-averaged measurements, thus limiting the information derivable from the data. The dependence of such fixed-in-space angular distributions on photon energy provides an exciting new probe of electronic structure and dynamics. With our new method we can accurately calculate the angular distributions of photoelectrons emitted from core levels of small molecules with definite orientations in space. The results are found to be in excellent agreement with recent extensive sets of experimental data. The theory can also be applied to the study of other more complex problems as well, as for example in the study of low-energy photoemission and photoelectron diffraction processes from the valence band of low-symmetry systems (such as clusters and adsorbates), for which the application of standard one-step models is problematic.

Dr. I. Skliadneva

Russian Academy of Sciences, Tomsk, Russia
05-04 through 30-06-2002
Phonon spectra in bulk metals and at metal surfaces.
Relaxation and phonon spectra of surface alloys of palladium on Cu(100) have been studied by using embedded atom method. The calculation showed complex character of the surface relaxation and very strong Pd-Cu interatomic interactions which explain the experimentally observed alloy surface phonon models. First-principles calculations have been done for phonon spectra of MgB2 to compare them with the recently measured spectra of this material. Very high frequency models obtained can explain the importance of the phonon contribution to the lifetime broadening of electron states in MgB2.

Dr. T. Strasser

Universität Kiel, Germany
03-08 through 29-11-2002
Photoelectron diffraction for electronic and structural characterization of solid crystal surfaces.
This visitor has used his expertise in calculating photoemission intensities from first principles in a one-step model approach to the case of aluminium (111) surfaces. His theory has permitted explaining recent experimental spectra that have resulted in the first accurate experimental determination of high-energy conduction bands in a solid surface. Part of his work during his stay at DIPC has been also devoted to the study of photoemission from stepped surfaces with full inclusion of multiple scattering. This part of his work is still underway.

Dr. T. Teperik

Russian Academy of Sciences, Saratov, Russia
02-11 through 22-12-2002
Optical response of metallic metamaterials
Description: The research of Dr. Teperik during his stay at San Sebastian was focused on understanding the behaviour of light in interaction with metallic metamaterials composed of subwavelength air inclusions in silver, gold, and other metals. Her calculations showed that the reflectivity from the surfaces of this type of materials exhibits strong reflection and transmission resonances that can be attributed either to localized Mie modes of the inclusions or to Bragg reflections in the case of ordered arrays of inclusions. This is an ongoing work, and actually, Dr. Teperik is now progressing in the understanding of these materials while she continues performing calculations from Saratov.

Short Visits

Dr. M. Aeschlimann
Universität Essen, Germany
08-03 through 11-03-2003
Ultrafast two-photon photoemission studies of excited electrons in metals.

Prof. M. Aguila
CIEMAT-CSIC, Spain
11-07 through 14-07-2002
Particle physics: current status and perspectives.

Dr. R. Aguado
ICMM-CSIC, Spain
09-05 through 09-05-2003
Kondo effect in quantum dots.

Prof. F. Agulló
Universidad Autónoma de Madrid, Spain
04-09 through 06-09-2002
Ion beam tecniques in the analysis of materials.

Dr. J. Aizpurua
National Institute of Standards and Technology (NIST), Gaithersburg, USA
05-09 through 05-09-2002
Tunnel-coupled quantum dots : Atomistic Theory of Quantum Dot Molecules ans Arrays.

Prof. P.M. Ajayan
Rensselaer Polytechnic Institute, New York, USA
12-06 through 15-06-2002
Synthesis, Mechanical and electronic properties of carbon nanotubes and their assemblies.

Prof. C. Alejaldre Losilla
CIEMAT, CSIC, Spain
28-02 through 28-02-2003
Fusion energy and the ITER project: present situation and future perspectives.

Prof. J. Alonso
Universidad de Valladolid, Spain
10-05 through 13-05-2002
Hydrogen adsorption in carbon nanotubes.

Dr. F. Aryasetiawan
Research Institute for Computational Science (RICS), Japan
13-01 through 20-01-2002
Total energy method from many-body formulation.

Prof. M.C. Asensio
C. LURE, France - ICMM-CSIC, Madrid, Spain
17-02 through 20-02-2002
Fermi Surface Mapping of 2-D and 3-D Systems by Angle Resolved Photoemission.

Prof. Dr. N.W. Ashcroft
Cornell University, Ithaca, New YorK, USA
26-03 through 17-04-2002 and 11-06 through 07-2003
Theory of Many Particle Systems, Density Fuctional, Theory (Classical and Quantum), and Theory of Dense Hydrogen and Matter under Extreme Conditions.

Prof. R. Baragiola
University of Virginia, Charlottesville, USA
01-04 through 03-04-2003
Electronic excitacion of insulating materials by slow ions: overview and the MgO case.

Dr. N. Barberán Falcón
Universidad de Barcelona, Spain
26-10 through 28-10-2003
Nanostructures under magnetic fields.

Prof. S. Baroni
SISSA and INFM DEMOCRITOS National Simulation Center, Trieste, Italy
09-11 through 11-11-2003
Monte Carlo simulation of the dynamics of quantum interacting systems: Structure, dynamics, and superfluidicity of small doped He clusters.

Dr. A. Bauer
Freie Universität Berlin, Germany
20-02 through 25-02-2002
Electronic Structure and Lifetimes of Surface States on Lanthanide Metals.

Prof. M.C. Bellissent-Funel
CNRS, Laboratoire Leon Brillouin LLB, Saclay, France
09-01 through 12-01-2003
Protein dynamics studied by Neutron Scattering and Molecular Dynamics Simulations.

Prof. G. Benedek
Universitaí degli Studi di Milano - Bicocca, Italy
22-11 through 26-11-2002
Surface phonons and phase transitions.

Prof. G.F. Bertsch
Editor Review of Modern Physics
University of Washington, USA
01-11 through 10-11-2002
Optical response of nanostructures.

Dr. G. Bihlmayer
IFF-FZ, Forschungszentrum Jülich, Germany
17-05 through 23-05-2003
Magnetism in low dimensions: Overlayers, wires and atoms.

Prof. J. Blanco
Universidad de Oviedo, Spain
05-06 through 06-06-2002
Neutron Scattering.

Prof. S. Blügel
Forschungszentrum Jülich, Germany
12-11 through 15-11-2002 and 14-12 through 18-12-2003
Magnetism at the Nanocosmos.
Rashba spin-orbit effect at metal surfaces.

Dr. M. Bode
Universität Hamburg, Germany
16-07 through 21-07-2003
Atomic resolution in magnetic STM.

Prof. D. Boerma
Universidad Autónoma de Madrid, Spain
03-09 through 06-09-2002
Atomic Collisions in Solids. Surface Physics and Computer Simulations.

Dr. A. Borisov
Université Paris Sud, France
04-05 through 31-05-2002, 01-12 through 05-12-2002 and 22-11 through 29-11-2003
Time Dependent Density Functional Theory of screening in metallic clusters.
Building up the screening below the femtosecond scale.

Dr. I. Boustani
Universität Wuppertal, Germany
15-08 through 15-09-2003
Boron quasiplanar clusters and nanotubes. From theoretical predictions to experimental confirmations.

J. Bravo Abad
Universidad Autónoma Madrid, Spain
09-10 through 10-10-2002
Superprism effect in photonic crystals.

Prof. L. Brey
ICMM-CSIC, Spain
23-01 through 24-01-2003
A lattice spin mechanism for colossal magnetoresistance in manganites.

Dr. T. Brixner
University of California, Berkeley, USA
03-12 through 07-12-2003
Adaptive Quantum Control: Technique and Applications

Dr. D. Cangialosi
University of Delft, The Netherlands
16-11 through 17-11-2003
Positron annihilation lifetime spectroscopy to study the dynamics of policarbonate far below Tg.

Dr. M.A. Cazalilla
ICTP. Trieste, Italy
09-01 through 12-01-2002, 04-06 through 06-06-2002, 09-07 through 12-07-2002 and 16-12 through 20-12-2002
Strongly correlated systems.
Some scenarios for strong correlation phenomena in ultracold atom systems.

Dr. S. Cerveny
Chalmers University of Technology, Sweden
07-12 through 15-12-2003
General framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other experimental techniques and MD-simulations.

Dr. A. Climent Font
Universidad Autónoma de Madrid, Spain
04-09 through 06-09-2002
Interaction of Energetic Ions with Solids, RBS and ERDA techniques.

Prof. E. Coronado Miralles
Universidad de Valencia, Spain
25-04 through 26-04-2002
Materiales Moleculares Multifuncionales.

Prof. V. Crespi
University of Pennsylvania, USA
30-05 through 02-06-2002
Electronical and mechanical properties of nanotubes.

A. Chauty
Université de Paris-Sud, France
29-07 through 30-07-2002
Effect of the hydrostatic pressure on the dynamics of polymer materials.

Prof. M. Dähne
Technische Universität Berlin, Germany
01-04 through 06-04-2002
Quantum dots and nanowires of rare-earth silicides studied with STM.

Prof. P. de Andres
ICMM-CSIC, Spain
21-11 through 22-11-2002
How do water molecules bind to close-packed metal surfaces?

Prof. P. Dederichs
Forschungszentrum Jülich, Germany
09-11 through 15-11-2002
Diluted Magnetic Seminconductors.

Prof. B. Deloche
Université Paris-Sud, France
07-05 through 09-05-2002, 19-02 through 23-02-2003, 13-07 through 15-07-2003 and 27-08 through 29-08-2003
Dynamics of Polymers in confined geometries.

Dr. A. Dereszewska
Merchant Maritime University, Gdynia, Poland
06-09 through 06-10-2002
Dielectrico relaxation of semirigid polymers in polar solvents. (Phase Transitions in Liquid Crystalline Polymer Solutions by means of Dielectric Spectroscopy)

Dr. L. Despont
Université de Neuchâtel, Switzerland
11-11 through 14-11-2003
Photoelectron diffraction: structural studies of surface reconstruction of ferroelectrics and implications on spontaneous polarization.

Dr. D. Dickerscheid
Universtiteit Utrecht, Holland
05-08 through 20-08-2003
Cold atoms bose-Einstain condensation in cold atoms systems and optical lattices.

Prof. J. Dobson
Griffith University, Australia
14-09 through 28-09-2003
Van der Walls interactions at leisure.

Prof. T.W. Ebbesen
Université Louis Pasteur, Strasbourg, France
24-10 through 27-10-2002
Extraordinary transmission through subwavelength holes.

Prof. T. Fauster
Lehrstuhl für Festkörperphysik, Erlangen, Germany
21-07 through 24-07-2003
Inter- and intraband scattering by defects at metal surfaces.

Prof. J. Fink
Institute for Solid State Research. IFW. Dresden, Germany
27-11 through 01-12-2002
Plasmons in solids studied by electron energy-loss spectroscopy.

Dr. V. Franco Puntes
Universidad de Barcelona, Spain
18-03 through 21-03-2003
Nanoparticles: Building units and built structures.

Dr. L.S. Froufe Pérez
Universidad Autónoma de Madrid, Spain
01-06 through 08-06-2003
Conductance Distributions in Disordered Wires at the Metal-Insulator Crossover.

Prof. A. Galindo
Universidad Complutense Madrid, Spain
30-09 through 01-10-2003
Quantum information and quantum algorithms. Basic problems in Quantum Physics. Completion of a two-volume textbook on Advanced Quantum Mechanics, and a textbook on Space-Time Structure.

Dr. A. García Arribas
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
07-11 through 07-11-2003
Effective-Hamiltonian Simulations in Ferroelectrics

Prof. F. García Moliner
Universitat Jaume I, Castellón, Spain
02-10 through 04-10-2003
The practical value of culture.

Prof. M.E. García
Frei Universität Berlin, Germany
15-02 through 15-02-2002
Laser induced ultrafast phase transitions.

Prof. J. Gómez
Universidad Autónoma de Madrid, Spain
28-02 through 01-03-2002
Microsocopía de proximidad: los ojos de la nanotecnología.

Prof. J.C. Gómez Sal
Universidad de Cantabria, Spain
05-06 through 06-06-2002
About non Fermi liquids and the cuantic phase of transitions in metals. An experimental approach.

Dr. M. Grüning
Universiteit van Amsterdam, The Netherlands
11-08 through 12-08-2003
Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

Prof. F. Guinea López
ICMM-CSIC, Spain
08-10 through 12-10-2003
Suppression of Quantum features and decay processes induced by metallic environments.

Prof. B. Hellsing
Chalmers and Göteborgs University, Sweden
22-04 through 28-04-2002, 17-11 through 24-11-2002 and 01-07 through 31-07-2003
Electron-phonon interactions on metal surfaces.
The influence of the electron-phonon coupling on lifetimes of excited elecron and hole states.

Prof. A. Hernando
Universidad Complutense de Madrid, Spain
30-09 through 01-10-2002
Magnetism of nanocristaline iron.

Prof. F. Himpsel
University of Wisconsin, Madison, USA
11-07 through 18-07-2002
Au and Ag nanostructures and atom chains on Si surfaces.

Dr. A.F. Ho
University of Birmingham, U.K.
01-03 through 30-03-2003
Effects of disorder in one-dimensional quantum liquids, and phase diagram of binary mixtures of one-dimensional harmonic fluids.

Dr. W.A. Hofer
University of Liverpool, U.K.
15-01 through 17-01-2003
Theory of scanning tunnelling microscopy.

Prof. P. Hofmann
University of Aarhus, Denmark
04-12 through 08-12-2002
Geometry, electronic structure and electron-phonon coupling on Bi surfaces.

Prof. K. Horn
Fritz-Haber- Institut Berlin, Germany
04-05 through 07-05-2002
High resolution photoemission spectroscopy from nanostructures.

Prof. I. Howard
Universiteit Antwerpen, Belgium
05-06 through 19-06-2003
Structural properties of small clusters with DFT techniques.

Prof. A. Howie
Cavendish Laboratory, Cambridge, U.K.
10-09 through 24-09-2002, 04-07 through 12-07-2003 and 03-09 through 17-09-2003
Physics of electron microscopy, including elastic and inelastic scattering of electrons, electron interference and electron energy loss spectroscopy, secondary electron emission and ionisation damage. Surface science, catalyst particles, crystal defects and solid state excitations.
Theory of valence electron excitations by fast electrons.

Prof. S. Iijima
Meijo University, Japan
11-04 through 13-04-2002
Carbon nanostructures: nanotubes, onions, cones.

Dr. A. Kazanskiy
University of St. Petersburg, Russia
14-05 through 15-05-2003
Electron dynamics at adsorbates on metals.

Dr. C. Kollath
Lehrstuhl für Theoretische Festkoerperphysik, München, Germany
04-11 through 01-12-2003
Ultra cold atoms optical lattices non equilibrium phenomena and Bose-Fermi mixtures.

Prof. E. Krasovskii
Universität Kiel, Germany
09-05 through 13-05-2002, 08-07 through 05-08-2002,
27-11 through 02-12-2002 and 04-08 through 29-08-2003
First-principles calculations of collective excitations in bulk metals.
Electronic structura and dielectric properties of heavy metals: Bi, La, and Lu.
Dielectris properties and collective excitations in heavy metals.

O. Krupin
Free Universität Berlin, Germany
13-01 through 25-01-2003
Structural and electronic studies using photoelectron diffraction from solid surfaces.

Dr. J. Kuntze
Universität Kiel, Germany
22-09 through 29-09-2003
"One-dimensional atom chains"
We have started a new project focused on the structural properties of one-dimensional Au atom chains grown on Si(111) vicinal surfaces. Such atomic chains are potential candidates to exhibit one-dimensional Luttinger liquid behaviour. Previous experiments display exotic properties, like fractional band filling. Moreover, they are expected to undergo a structural charge-density wave transition at low temperature, which could be directly observed at our STM chamber.

Prof. Dr. V. Kuznetsov
Tomsk State University, Russia
06-04 through 04-05-2002
Density functional methods in the theory of phase diagrams of alloys and in the Kondo effects.

Dr. N. Lorente
Université Paul Sabatier, Toulouse, France
16-10 through 17-10-2002
Controlled reactions on single molecules on surfaces.

Prof. E. Ludeña
IVIC, Caracas, Venezuela & Universidad Autónoma de Madrid, Spain
25-06 through 29-06-2003
Is DFT a semi-empirical theory? Somme comments on its foundations, accomplishments and shortcomings.

Dr. R. Magyar
Rutgers University, USA
16-03 through 19-03-2003
Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

Prof. N.H. March
Universiteit Antwerpen, Belgium
01-11 through 30-11-2002 and 28-05 through 25-06-2003
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.
Correlation functionals in DFT.

Prof. M. Mareschal
CECAM, ENS-Lyon, France
29-04 through 29-04-2002
Statistical mechanics applied to granular materials and polymers.

Dr.C. Marinica
CNRS, Laboratoire des Collisions Atomiques et Moléculaires, Orsay, France
22-01 through 25-01-2003
Electron excitations at metal surfaces covered with noble gas atoms.

Prof.R. Matzdorf
Universität Würzburg, Germany
23-10 through 28-10-2003
Electron correlations and electron-phonon coupling in adsorbates on noble-metal surfaces.

Prof. F.J. Meseguer
Unidad Asociada CSIC - UPV, Física Aplicada, Spain
04-03 through 05-03-2002
Photonic crystals and related structures.

Prof. J.E. Miraglia
IAFE and Universidad de Buenos Aires, Argentina
16-09 through 16-09-2003
Plasmon Decay and Nonlinear Effects.

Prof. R. Miranda
Universidad Autónoma de Madrid, Spain
26-05 through 27-05-2003
Tunnelling Spectroscopy on metallic nanostructures: observing the electronic states of confined systems.

Dr. P. Molinás i Mata
Universidad Politécnica de Catalunya, Spain
22-04 through 22-04-2003
"Two-dimensional diffusion of vacants on Ge(111) surfaces"
Atomic defects at Ge(111) surfaces display a rich, temperature diffusion behaviour. They act as single particles with isotropic or anisotropic diffusion, depending on temperature and vacant concentration. In this project we prepare highly perfect Ge surfaces and create vacants with the STM tip. The diffusion properties of such vacants will be studied as a function of temperature.

Prof. G. Morata
Centro Biología Molecular - Universidad Autónoma Madrid, Spain
23-09 through 23-09-2002
Science and Society at the dawn of the XXI Century - Social Impact of Biological Techniques.

Prof. R. Mukhopadhyay
Solid State Physics Division, BARC, India
10-11 through 13-11-2003
Stochastic Dynamics in Condensed Matter: Neutron Scattering Study.

Prof. I. Nagy
Technical University Budapest, Hungary
03-01 through 01-02-2002
Spin effects in electron lifetimes.

Prof. V. Nazarov
Kyushu Institute of Technology, Kitakyushu, Japan
11-07 through 10-08-2002 and 09-02 through 07-03-2003
Bulk and surfaces plasmons.
Collective excitations in bulk metals and at their surfaces.

Dr. M. Neeb
BESSY Cmbh, Berlin, Germany
19-02 through 23-02-2003
Ultrafast relaxation dynamics of optically excited states in small transition metal clusters.

Dr. P. Ordejón
ICMAB-CSIC, Spain
08-04 through 12-04-2003
First principles calculations of ballistic transport in nanoscale systems.

Dr. J. Ortega Mateo
Universidad Autónoma de Madrid, Spain
08-11 through 09-11-2002
Dynamical fluctuations and the sqrt(3)xsqrt(3) —> 3x3 transition in alpha—Sn/Ge(111) and Sn/Si(111).

Dr. R. Otero
STM de Miranda, Madrid, Spain
18-02 through 01-03-2002
Ag-Au stripes and lateral superlattices.

Dr. J.J. Palacios
Universidad de Alicante, Spain
21-03 through 22-03-2002
Molecular electronics from first principles.

Dr. I. Pascual
ICMAB-CSIC, Spain
19-12 through 22-12-2002
STM in lateral nanostructures.

Prof. J. Pendry
Imperial College London, U.K.
12-05 through 16-05-2003
The Perfect Lens - Focusing Beyond the Diffraction Limit.

Prof. J. Perdew
University of Tulane, New Orleans, USA
13-07 through 19-07-2003
Climbing Jacob's Ladder: The Meta-Generalized Gradient Approximation for Exchange and Correlation.

Dr. W. Pfeiffer
Universität Würzburg, Germany
18-09 through 22-09-2002
Electron Dynamics in Supported Nanoparticles.

Prof. G. Platero Coello
Universidad Autónoma de Madrid, Spain
04-12 through 05-12-2003
Dynamical control of electronic states in AC-Driven Quantum Dots

Prof. V. Ponce
Centro Atómico Bariloche, Argentina
02-06 through 28-06-2002 and 02-06 through 30-06-2003
Electron emission in the interaction of light ions with surfaces.
Atomic Collisions In Solids. Ion-surface Interactions.

Dr. S. Reich
Technische Universität Berlin, Germany
14-07 through 20-07-2003
Espectroscopia vibracional y absorción óptica en nanotubos y otros compuestos de carbono.

Dr. F. Reinert
Universität des Saarlander, Saarbrücken, Germany
18-04 through 21-04-2002
Photoemission study of the hole dynamics in surface states.

Prof. D. Richter
IFF-FZ, Forschungszentrum Jülich, Germany
07-07 through 14-07-2002 and 25-06 through 14-07-2003
Polymer dynamics by neutron techniques.

Prof. A. Salin
Université de Bordeaux I, France
28-01 through 29-01-2002 and 03-02 through 04-02-2003
Dissociation dynamics of diatronic molecules at metal surfaces.

Dr. F. Schiller
Universität Dresden, Germany
24-04 through 29-04-2003
Crystalline and electronic structure of thin Be and Mg films.

Dr. A. Schneider
Max-Planck-Institut FKF, Stuttgart, Germany
17-04 through 19-04-2002
Scanning tunneling microscopy study of surface states.

Prof. W.D. Schneider
Université de Lausanne, Switzerland
10-10 through 13-10-2002
Scanning tunneling spectroscopy and microscopy of nanostructures.

Dr. W.D. Schoene
Free Universität Berlin, Germany
11-01 through 15-01-2003, 31-07 through 30-08-2003 and
14-12 through 18-12-2003
Lifetimes of excited electrons in metals.
Calculating quasiparticle energies in different approximations.
Many-body GW calculations of electronic structure and quasiparticle lifetimes in metals.

Dr. G. Schwartz
Chalmers University of Technology, Sweden
07-12 through 15-12-2003
General framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other experimental techniques and MD-simulations.

Dr. J. Sjakste
Université Paris-Sud, France
08-09 through 09-09-2003
Electronic transfer in the interaction of ions with surfaces.

Prof. J.M. Soler Torroja
Universidad Autónoma de Madrid, Spain
31-01 through 01-02-2002
The SIESTA method for ab initio order-N materials simulation.

Prof. P. Soukiassian
Commissariat a l'Energie Atomique, Saclay, France
05-11 through 08-11-2002
Silicon carbide surfaces and nanostructures.

Prof. M.J. Stott
Queen's University, Kingston, Ontario, Canada
13-07 through 16-07-2003
Modelling Bioactive Calcium Phosphate Ceramics.

Prof. J. Tejada Palacios
Universidad de Barcelona, Spain
22-10 through 24-10-2003
Resonant spin tunnelling and related phenomena.

Prof. S. Tretyakov
Helsinki University of Technology, Finland
03-02 through 05-02-2003
Microwave technology and electron magnetic band gap materials.

Prof. J.M. Ugalde Uribe-Etxebarria
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
14-02 through 14-02-2003
An innocent chemist look at the Density Functional Theory.

S. Vaccaro
EPFL Lausanne, Switzerland
03-02 through 04-02-2003
Optical metamaterials in microwave technology.

Prof. V.R. Velasco
ICMM-CSIC, Spain
12-12 through 13-12-2002
Physical properties of quasi-periodic systems. Dreams and realities.

Prof. L. Viña
Universidad Autónoma de Madrid, Spain
31-01-2002 through 31-01-2003 and 30-05 through 30-05-2003
Semiconductor quantum microcavities: a solid state approach for condensation.

Prof. U. Von Barth
Lunds Universitet, Sweden
19-10 through 23-10-2002
Density functional theory and many-body approaches for exchange and correlation functionals.

Dr. M. Wierzbowska
Trinity College, Dublin, Ireland
16-06 through 06-07-2003
Ab-initio calculations in dilute magnetic semiconductors. Description of components based on GaN by means of an LDA+U approach.

Prof. H. Winter
Technische Universität Wien, Austria
30-05 through 21-06-2002
Molecular projectile effects for kinetic electron emission from carbon- and metal surfaces bombarded by slow hydrogen ions.

Prof. H. Winter
Universität zu Berlin, Germany
15-06 through 18-06-2002
Charge exchange, energy loss and electron emission in Ion-Surface Collisions.

Prof. E. Zaremba
Queen's University, Canada
21-07 through 06-08-2002
Bose-Eisntein Condensate.

Dr. I. Zozoulenko
University of Linkoeping, Sweden
05-09 through 06-09-2003
Wave and ray dynamics in optical cavities and quantum electron billiards.

THE SEMINARS

DIPC offers a full program of seminars by acclaimed authorities in the field.

02

F. Aryasetiawan
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F. J. Meseguer
J. J. Palacios
M. Dähne
S. Iijima
N. W. Ashcroft
A. Schneider
F. Reinert
E. Coronado Miralles
M. Mareschal
V. Kuznetsov
K. Horn
J. Alonso
V. Crespi
J. C. Gómez Sal
P. M. Ajayan
H. Winter
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M. Aguilar
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J. Aizpurua
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T. W. Ebbesen
P. Soukiassian
J. Ortega Mateo
P. Dederichs
S. Blügel
N. H. March
A. Kaminskii
P. de Andrés
G. Benedek
E. Krasovskii
T. Strasser
J. Fink
P. Hofmann
V. R. Velasco
I. Pascual

Invited Speakers

03

M.C. Bellissent-Funel
W. Schoene
C. Lemell
C. Marinica
L. Brey
L. Viña
J.M. Ugalde Uribe-Etxebarria
M. Neeb
C. Alejaldre Losilla
A.F. Ho
M. Aeschlimann
V.F. Puntes
R. Baragiola
P. Ordejón
F. Schiller
R. Aguado
J.B. Pendry
G. Bihlmayer
R. Miranda
L. Viña
L. Salvador Froufe
E.V. Ludena
N.W. Ashcroft
M.J. Stott
J. P. Perdew
M. Bode
T. Fauster
W. Schoene
I. Boustani
I. Zozoulenko Linkoeping
J.E. Miraglia
J. Dobson
F. García Moliner
F. Guinea
J. Tejada
R. Matzdorf
N. Barberan
A. García
S. Baroni
R. Mukhopadhyay
D. Cangialosi
T. Brixner
G. Platero
S. Bluge

02

Seminars 2002

JANUARY 18, 2002

Total energy method from many-body formulation

F. Aryasetiawan (National Institute of Advanced Industrial Science and Technology, Japan)

FEBRUARY 1, 2002

The SIESTA method for ab initio order-N materials simulation

J. M. Soler Torroja (Universidad Autónoma de Madrid, Spain)

FEBRUARY 15, 2002

Laser induced ultrafast phase transitions

M. E. García (Frei Universität Berlin, Germany)

FEBRUARY 19, 2002

Fermi Surface Mapping of 2-D and 3-D Systems by Angle Resolved Photoemission

M. C. Asensio (LURE, Paris, France/ICMM-CSIC, Madrid, Spain)

FEBRUARY 21, 2002

Dephasing of optically excited electron-hole pairs in 2-D bands of the image potential

B. Gumhalter (University of Zagreb, Croatia)

FEBRUARY 22, 2002

Electronic Structure and Lifetimes of Surface States on Lanthanide Metals

A. Bauer (Freie Universität Berlin, Germany)

MARCH 1, 2002

Microsocopía de proximidad: los ojos de la nanotecnología

J. Gómez (Universidad Autónoma de Madrid, Spain)

MARCH 5, 2002

Cristales fotónicos y estructuras relacionadas-Photonic crystals and related structures

F. J. Meseguer (Unidad Asociada CSIC - Universidad Politécnica de Valencia, Spain)

MARCH 22, 2002

Electrónica molecular desde primeros principios/Molecular electronics from first principles

J. J. Palacios (Unidad Asociada CSIC - Universidad de Alicante, Spain)

APRIL 5, 2002

Structure and optical properties of self-organized semiconductor nanostructures

M. Dähne (Technische Universität Berlin, Germany)

APRIL 12, 2002

Past, present, and future of carbon nanotubes

S. Iijima (Meijo University, Japan)

APRIL 16, 2002

Complexity in the hitherto simple metals

N. W. Ashcroft (Cornell University, New York, USA)

APRIL 18, 2002

Kondo resonance and STM: Probing the interaction of a Single Magnetic Atom with Bulk and Surface electrons

A. Schneider (Max-Planck-Institüt FKF, Stuttgart, Germany)

APRIL 19, 2002

Direct observation of low-energy features in the photoemission spectra of conventional superconductors and heavy-ferminons compounds

F. Reinert (Universität des Saarlander, Saarbrücken, Germany)

APRIL 26, 2002

Materiales Moleculares Multifuncionales

E. Coronado Miralles (Universidad de Valencia, Spain)

APRIL 29, 2002

What is the difference between a fluid and a granular fluid?

M. Mareschal (CECAM, ENS-LYON, France)

MAY 3, 2002

Local magnetic moment interaction problem revisited: The role of electron kinetic energy in magnetic interactions en metals

V. Kuznetsov (Physics Faculty, Tomsk State University, Russia)

MAY 6, 2002

Electronic structure in low-dimensional systems and complex quasicrystalline alloys

K. Horn (Fritz-Haber- Institüt, Berlin, Germany)

MAY 13, 2002

Absorción de hidrógeno en nanotubos de carbono

J. Alonso (Universidad de Valladolid, Spain)

MAY 31, 2002

Theory of nanostructures: Boron-based nanotubes, nanocones, perfect bearings, the strongest nanotubes, and magnetic hurricanesin ordered porous magnets

V. Crespi (University Park, Pennsylvania, USA)

JUNE 6, 2002

Sobre los líquidos no de Fermi y las transiciones de fase cuánticas en metales. Una aproximación experimental

J. C. Gómez Sal (Universidad de Cantabria, Spain)

JUNE 14, 2002

Organized Assembly of Carbon Nanotube Architectures

P. M. Ajayan (Rensselaer Polytechnic Institute, New York, USA)

JUNE 17, 2002

Auger neutralization of He+ ions in front of Ag(111)

H. Winter (Humboldt-Universität zu Berlin, Germany)

JUNE 18, 2002

Future Energy from Thermonuclear Fusion: Scientifically possible? Technologically feasible? Socioeconomically acceptable?

H. Winter (Technische Universität Wien, Austria)

JULY 11, 2002

Some scenarios for strong correlation phenomena in ultracold atom systems

M. A. Cazalilla Gutierrez (ICTP, Trieste, Italy)

JULY 12, 2002

Física de partículas: estatus y perspectivas

M. Aguilar (CIEMAT, Madrid, Spain)

AUGUST 5, 2002

Dynamics of Bose-Einstein Condensed Gases at Finite Temperatures

E. Zaremba (Queen's University, Canada)

SEPTEMBER 4, 2002

Las técnicas de haces de iones para el análisis de materiales: El Centro UAM

F. Agulló (Universidad Autónoma de Madrid, Spain)

SEPTEMBER 5, 2002

Tunnel-coupled quantum dots: Atomistic Theory of Quantum Dot Molecules and Arrays

J. Aizpurua (NIST, Gaithersburg, USA)

SEPTEMBER 19, 2002

Electron Dynamics in Supported Nanoparticles

W. Pfeiffer (Universität Wuerzburg, Germany)

SEPTEMBER 24, 2002

Growth of Cobalt silicides on Si(111) and vicinal Si(111)

M. Löffler (Lehrstuhl für Festkärperphysik, Erlangen, Germany)

SEPTEMBER 30, 2002

Determinación de movilidad molecular de polímeros semirígidos por medio de espectroscopia dieléctrica

A. Dereszewska (Merchant Maritime University, Gdynia, Poland)

OCTOBER 1, 2002

Magnetismo del hierro nanocristalino

A. Hernando (Universidad Complutense de Madrid, Spain)

OCTOBER 7, 2002

Challenges and Errors: Interpreting high resolution Images of scanning tunneling microscopes

W. A. Hofer (University College London, England)

OCTOBER 11, 2002

Scanning tunneling spectroscopy and microscopy of nanostructures

W. Schneider (Université de Lausanne, Switzerland)

OCTOBER 17, 2002

Controlled reactions on single molecules on surfaces

N. Lorente (Université Paul Sabatier, Toulouse, France)

OCTOBER 25, 2002

Diffraction Control and Enhanced Transmission through Sub-Wavelength Apertures in Metal Films

T. W. Ebbesen (Université Louis Pasteur, Strasbourg, France)

NOVEMBER 6, 2002

Atomic Control of Silicon Carbide Surfaces and Highly Stable Nanostructures

P. Soukiassian (Commissariat de l'Energie Atomique, Saclay, DSM-DRECAM-SPCSI-SIMA, France)

NOVEMBER 8, 2002

Dynamical fluctuations and the sqrt(3)xsqrt(3) —> 3x3 transition in alpha—Sn/Ge(111) and Sn/Si(111)

J. Ortega Mateo (Universidad Autónoma de Madrid, Spain)

NOVEMBER 11, 2002

Diluted Magnetic Seminconductors

P. Dederichs (Forschungszentrum Jülich, Germany)

NOVEMBER 13, 2002

Magnetism at the Nanocosmos

S. Blügel (Forschungszentrum Jülich, Germany)

NOVEMBER 14, 2002

Fingerprints of unconventional superconductiviry in heavy Fermion materials and high Tc cuprates

N. H. March (Universiteit Antwerp, RUCA, Antwerp, Belgium)

NOVEMBER 18, 2002

Novel nonlinear-laser xsi(2)- and xsi(3)-active crystals and new self-frequency conversion effects

A. Kaminskii (Russian Academy of Sciences, Russia)

NOVEMBER 22, 2002

How do water molecules bind to close-packed metal surfaces?

P. de Andrés (ICMM-CSIC, Madrid, Spain)

NOVEMBER 25, 2002

Surface phonons and phase transitions

G. Benedek (Universitaí degli Studi di Milano - Bicocca, Italy)

NOVEMBER 28, 2002

Electronic structure and dielectric properties of Bi

E. Krasovskii (Universität Kiel, Germany)

NOVEMBER 28, 2002

One step photoemission calculation from a multiple scattering cluster-model approach

T. Strasser (Universität Kiel, Germany)

NOVEMBER 29, 2002

Plasmons in solids studied by electron energy-loss spectroscopy

J. Fink (Institute for Solid State Research, IFW, Dresden, Germany)

DECEMBER 5, 2002

Geometry, electronic structure and electron-phonon coupling on Bi surfaces

P. Hofmann (University of Aarhus, Denmark)

DECEMBER 13, 2002

Physical properties of quasi-periodic systems. Dreams and realities

V. R. Velasco (ICMM-CSIC, Madrid, Spain)

DECEMBER 20, 2002

STM in lateral nanostructures

I. Pascual (ICMB-CSIC, Barcelona, Spain)

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Seminars 2003

JANUARY 10, 2003

Protein dynamics studied by Neutron Scattering and Molecular Dynamics Simulations

M.C. Bellissent-Funel (CNRS, Laboratoire Leon Brillouin LLB, Saclay, France)

JANUARY 14, 2003

Lifetimes of excited electrons in metals

W. Schoene (Fritz-Haber-Institut der Max-Planck, Berlin, Germany)

JANUARY 17, 2003

Many Electron Systems Interacting with Strong Fields

C. Lemell (University of Technology, Vienna, Austria).

JANUARY 23, 2003

Quantum-well resonances and image states in the Ar/Cu(100) system

C. Marinica (Laboratoire des Collisions Atomiques et Moleculaires, Paris, France)

JANUARY 24, 2003

A lattice spin mechanism for colossal magnetoresistance in manganites

L. Brey (ICMM-CSIC, Madrid, Spain)

JANUARY 31, 2003

Semiconductor quantum microcavities: a solid state approach for condensation

L. Viña (Universidad Autónoma de Madrid, Spain)

FEBRUARY 14, 2003

An innocent chemist look at the Density Functional Theory

J.M. Ugalde Uribe-Etxebarria (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)

FEBRUARY 21, 2003

Ultrafast relaxation dynamics of optically excited states insmall transition metal cluster

M. Neeb (BESSY GmbH, Berlin, Germany)

FEBRUARY 28, 2003

Fusion energy and the ITER project: present situation and future perspectives

C. Alejaldre Losilla (Laboratorio Nacional de Fusión, CIEMAT, Madrid, Spain)

MARCH 03, 2003 AND MARCH 04, 2003

Two lectures on basic Kondo physics

A.F. Ho (University of Birmingham, UK)

MARCH 10, 2003

Ultrafast two-photon photoemission studies of excited electrons in metals

M. Aeschlimann (University of Essen, Germany)

MARCH 21, 2003

Nanoparticles: Building Units and Built Structures

V.F. Puntes (Universidad de Barcelona, Spain)

MARCH 21, 2003

Excitación electrónica de aislantes por iones lentos: generalidades y el caso del MgO

R. Baragiola (Virginia, Charlottesville, USA)

APRIL 10, 2003

First principles calculations of ballistic transport in nanoscale systems

P. Ordejón (ICMB-CSIC, Barcelona, Spain)

APRIL 28, 2003

Crystalline and electronic structure of thin Be and Mg films

F. Schiller (Institut für Oberflaechen-und Mikrostrukturphysik TU- Dresden, Germany)

MAY 09, 2003

Kondo effect in quantum dots

R. Aguado (ICMM-CSIC, Madrid, Spain)

MAY 13, 2003

The Perfect Lens - Focusing Beyond the Diffraction Limit

J.B. Pendry (Imperial College, London, UK)

MAY 21, 2003

Magnetism in low dimensions: Overlayers, wires, and atoms

G. Bihlmayer (Institute for Solid State Physics, Jülich, Germany)

MAY 27, 2003

Tunneling Spectroscopy on metallic nanostructures: Observing the electronic states of confined systems

R. Miranda (Universidad Autónoma de Madrid, Spain)

MAY 30, 2003

Semiconductor quantum microcavities:a solid state approach for condensation

L. Viña (Universidad Autónoma de Madrid, Spain)

JUNE 03, 2003

Conductance Distributions in Disordered Wiresat the Metal-Insulator Crossover

L. Salvador Froufe (Universidad Autónoma de Madrid, Spain)

JUNE 27, 2003

Is DFT a semi-empirical theory? Some comments on its foundations, accomplishments and shortcomings

E.V. Ludena (IVIC Caracas, Venezuela and Universidad Autónoma de Madrid, Spain)

JULY 02, 2003

New ground state quantum liquids (accessible in the laboratory) in dense hydrogen and deuterium?

N.W. Ashcroft (Cornell University, New York, USA)

JULY 14, 2003

Modelling Bioactive Calcium Phosphate Ceramics

M.J. Stott (Queen's University, Kingston, Ontario, Canada)

JULY 18, 2003

Climbing Jacob's Ladder: The Meta-Generalized Gradient Approximation for Exchange and Correlation

J. P. Perdew (Tulane University, New Orleans, Lousiana, USA)

JULY 21, 2003

Atomic resolution in magnetic STM

M. Bode (Universität Hamburg, Germany)

JULY 24, 2003

Inter- and intraband scattering by defects at metal surfaces

T. Fauster (Universität Erlangen-Nurnberg, Germany)

AUGUST 20, 2003

Lifetimes of excited electrons in metals

W. Schoene (Free University Berlin, Germany)

SEPTEMBER 04, 2003

Boron quasiplanar clusters and nanotubes. From theoretical predictions to experimental confirmations

I. Boustani (Universität Wuppertal, Germany)

SEPTEMBER 05, 2003

Wave and Ray dynamics in optical cavities and quantum electron billiards

I. Zozoulenko (Linköpings Universitet, Sweden)

SEPTEMBER 16, 2003

Plasmon decay and nonlinear effects

J.E. Miraglia (IAFE and Universidad de Buenos Aires, Argentina)

SEPTEMBER 26, 2003

Van der Walls interactions at leisure

J. Dobson (Griffith University, Queensland, Australia)

OCTOBER 03, 2003

El valor práctico de la cultura

F. García Moliner (Universitat Jaume I, Castellón, Spain)

OCTOBER 10, 2003

Suppression of Quantum features and decay processes induced by metallic enviroments

F. Guinea (ICMM-CSIC, Madrid, Spain)

OCTOBER 23, 2003

Resonant spin tunneling and related phenomena

J. Tejada (Universidad de Barcelona, Spain)

OCTOBER 24, 2003

Electron correlations and electron-phonon coupling in adsorbates on noble-metal surfaces

R. Matzdorf (Universität Kassel, Germany)

OCTOBER 27, 2003

Nanostructures under magnetic fields

N. Barberan (Universidad de Barcelona, Spain)

NOVEMBER 07, 2003

Effective-Hamiltonian Simulations in Ferroelectrics

A. García (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)

NOVEMBER 11, 2003

Montecarlo simulation of the dynamics of quatum interacting systems: structure, dynamics and superfluidicity of small doped He clusters

S. Baroni (SISSA and INFM DEMOCRITOS National Simulation Center, Trieste, Italy)

NOVEMBER 11, 2003

Stochastic Dynamics in Condensed Matter: Neutron Scattering Study

R. Mukhopadhyay (BARC, Mumbai, India)

NOVEMBER 17, 2003

Positron annihilation lifetime spectroscopy to study the dynamics of policarbonate far below Tg

D. Cangialosi (University of Delft, Holland)

DECEMBER 04, 2003

Adaptive Quantum Control: Technique and Applications

T. Brixner (University of California, Berkeley, USA)

DECEMBER 05, 2003

Dynamical control of electronic states in AC-Driven Quantum Dots

G. Platero (ICMM-CSIC, Madrid, Spain)

DECEMBER 16, 2003

Rashba spin-orbit effect at metal surfaces

S. Blugel (IFF, Jülich, Germany)

THE WORKSHOPS

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

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Workshop 2002

Comelcan meeting and Workshop on Transport in Nanotubes

JUNE 3-7, 2002

Program Committee
Prof. P. M. Echenique (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)
Prof. A. Rubio (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)

The aim of this workshop is to review the recent advances in the physics of carbon nanotubes, addressing the applications in electron-mechanical devices and nanoelectronics. We address new features and techniques related to the electronic transport through these one-dimensional structures: superconductivity, electron-correlations, quantum coherence, ballistic and coulomb blockade effects, etc. The workshop is complemented with an internal meeting of the COMELCAN research training network as well as a young researchers meeting.

CONTRIBUTIONS

V. Krstic	**Ballistic and electron-correlated transport and other electrical transport phenomena in carbon nanotubes**
S. Guéron	**Superconductivity in carbon nanotubes**
T. Nussbaumer	**Superconductor-(NT) Quantum Dot-Superconductor or SNS junctions**
M. Grioni	**Fermi liquid versus Luttinger liquid in 1D systems: what do we learn from photoemission?**
S. Roche	**Quantum transport in carbon nanotube based systems**
O. Chauvet	**Transport properties on SWNT/PMMA**
S. Purcell	**Current-induced heating of carbon nanotubes during field emission: experiment and modelisation**

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Towards atomic scale- and time-resolution at interfaces

JULY 1-5, 2002

Program committee
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Prof. A. Goldmann (Universität Kassel, Germany)
Prof. U. Höfer (Philipps-Universität Marburg, Germany)
Prof. M. Wolf (FU Berlin, Germany)
Prof. W. Zinth (LMU München, Germany)

The aim of this workshop is to bring together researchers with backgrounds in theory and experiments in order to assess the present state of our understanding of ultrafast phenomena and atomic control at interfaces in condensed matter, surface science, chemistry, and biology. The idea is to contrast both theoretical and experimental studies to gain insight and establish new links and future collaborations.

CONTRIBUTIONS

July 1

K. Kern	**Scanning tunneling microscopy as local probe of electron density and dynamics**
R. Berndt	**Probing Electron Dynamics with STM**
K.-H. Rieder	**The scanning tunneling microscope as operative tool: Physics and chemistry with single atoms and molecules"**
Z.W. Gortel	**The core level clock in free molecules and in adsorbates**
W. Wurth	**Ultrafast charge transfer processes at adsorbates investigated using the core level clock**
D. Menzel	**Selective bond breaking in adsorbates by core excitations**
W. Zinth	**Femtosecond Processes in Primary Photosynthesis: Reactions Optimized for Highest Efficiency**

July 2

K. Morgenstern	**Electron-induced manipulation of water on surfaces: From hexamer formation to dissociation**
K. Reuter	**Surface knowledge from ultra-high vacuum to technically-relevant conditions: the example of catalytic CO oxidation**
A. González Ureña	**Laser induced charge - transfer processes at adsorbate/ metal interfaces**
M. Wolf	**Femtochemistry and ultrafast electron dynamics at adsorbate/metal interfaces**
M. Bonn	**Surface dynamics studied with femtosecond vibrational spectroscopy**
K. Al-Shamery	**Photoinduced processes at nanoparticulate systems**

July 3

G. Dujardin	**Atomic-scale control of electronic and dynamical processes on semiconductor and insulator surfaces**
F. Flores	**Inelastic mean free path for electrons : Ballistic Electron Emission Microscopy**
W.-D. Schneider	**Scanning tunneling spectroscopy and microscopy of ultrathin dielectric films**
U. Höfer	**Five-wave mixing investigation of electron dynamics at silicon surfaces**
W. Pfeiffer	**Ultrafast transport phenomena in metal-insulator-metal contacts**
H. Petek	**Ultrafast relaxation of electrons in metals in space, time, frequency domains**
T. Heinz	**Combining femtosecond lasers with Scanning Tunneling Microscopy**
A. Castro	**Optical Properties of nanostructures: a first-principle approach**

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July 4

M. Weinel (Th. Fauster)	**Femtosecond dynamics of electrons at surfaces**
J.-P. Gauyacq	**Effects of adsorbates on image states at metal surfaces**
H. Dürr	**Probing nanomagnetism on the femtosecond time scale**
S. Hufner	**Surface state width on noble metal (111) surfaces**
M. Persson	**Theory of single molecule vibrational spectroscopy and microscopy**
T. Frauenheim	**Towards theoretical understanding of nanoscale materials functioning and biomolecular processing**
E. Chulkov	**Momentum Resolved Electron and Phonon Contribution to the Quasiparticle Decay at Metal Surfaces**
A. Eiguren	**Electron phonon contribution to the lifetime of surface states**

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W. Wurth ..... Universität Hamburg, Germany
V. P. Zhukov ..... Donostia International Physics Center, Spain
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Reunión Nacional de Usuarios de Técnicas de Neutrones

OCTOBER 3-4, 2002

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Departamento de Física de Materiales (UPV/EHU)

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Dr. A. Arbe ("Unidad Física de Materiales", CSIC, Spain)
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Dr. J. Campo (ICMA-CSIC, Spain)

Chairman
Prof. J. Colmenero (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)

The main goal was the interchange of ideas, results and expertise among the Spanish neutron scattering users. On the other hand, with this conference – that is intended to be held each year or each two years – we tried to start a series of regular meetings within the Spanish neutron users community. The essence of this kind of conferences is the same as that of other similar meetings that take place periodically in other European countries, organized by the corresponding national associations included in the ENSA ("European Neutron Scattering Association").

CONTRIBUTIONS

J. Luzón
Study of the spin density distribution in the molecular magnet O2N.C6F4CNSSN by means of polarized neutron diffraction

J.M. de Teresa
Magnetic clusters in manganites probed with small-angle neutron diffraction

A. Señas
Pressure effects on TbM1-xCux (M=Pt and Ni) compounds

A. Arbe
Crossover from Gaussian to Non-Gaussian Behavior in the α-Relaxation of Polyisoprene

C. Cabrillo
Microscopic collective excitations in quantum and metallic liquids

A. Moreno
Methyl group dynamics in the disorder: from rotational tunneling to classical jump

G. Cuello
Neutron diffraction in liquid and amorphous systems

P. Monceau
Scientific activities at the Laboratoire Leon Brillouin (LLB) (Saclay, France)

Ch. Vettier
Fluctuations in Solids : neutrons provide a global view

R. Cywinski
Muon Beam Research in Condensed Matter Science: Achievements and Prospects

C. Frontera
Bismut effect on Manganites: a new mechanism for the charge order

D. Richter
Neutrons in Soft-Condensed Matter Science

M.A. González
Quasielastic neutron scattering in liquids with hydrogen bonds

P. Gorria
Study of crystallization kinetics and metastable phase segregation with neutron thermo-diffraction

M.A. Castro
Alkanes adsorption on graphite surface

F. Mezei
The ESS Revolution in Neutron Scattering Research Opportunities

J. Hernandez
Incommensurate Magnetic Structures in R2BaCoO5 Oxides (R=Rare Earth)

K. Clausen
ESS - the European project to maintain World leadership

S. García
Hydrogen bonds formation and structural stabilization in laminar and tridimensional phosphates

J.J. Blanco
Magnetic structure of the phases Sr2FeRe1-xBxO6 (B= Nb, Ta; x=0,0.1)

J.A. Alonso
Charge desproportion in the perovskites RniO3

cont'd

The participants on the grounds of Miramar Palace in San Sebastian

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03

Workshop 2003

Theoretical Biophysics Symposium

MARCH 5-7, 2003

Chairmen
Prof. J. M. Lluch (Universitat Autònoma de Barcelona, Spain)
Prof. L. A. Eriksson (Uppsala Universitet, Sweden)
Prof. J. Andres (Universitat Jaume I, Spain)
Prof. J. M. Ugalde (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)

Computers and computational methods have come to play an increasingly important role in natural sciences. In the area of biochemistry, theoretical modeling is for example used to understand the details governing why certain compounds or chemicals are toxic and others are not, how DNA is effected by UV-radiation, or how to design new and more efficient drugs.

During March 5 - 7, the Donostia International Physics Center (DIPC), along with the theoretical chemistry groups of The University of Uppsala and of the UPV/EHU, which are very active in these areas, organized a symposium on theoretical biochemistry/biophysics. The symposium brought together some 50 participants from Europe and North America, including many leading researchers in the field.

Among the many topics covered at the symposium were recent developments of the theoretical toolbox used by the researchers, as well as applications thereof to develop new antitumor drugs, to explain the toxicity of aluminium, or the intriguing fact that lobsters turn red upon cooking.

CONTRIBUTIONS

R. J. Boyd
Towards the development of theoretical models for biological catalysis

A. Largo
Synthetic routes for interstellar organic and prebiotic molecules

J. M. Mercero
Aluminum interactions with aminoacid side chains in a protein model environment

B. Durbeej
Some applications of time-dependent density functional methods to biochemical systems

J. Villa
Ion channels: through the hole and over the mountain

A. González-Lafont
On the location of stationary points in enzymatic catalysis: mandelate racemase as an example

J. I. Mujika
Theoretical study of the cleavage of the peptidic bond

R. Stole
Ligand binding and conformational changes in DNA gyrase B

V. Moliner
Theoretical insights in enzyme catalysis

N. Russo
A DFT investigation of some biomolecular systems

U. Ugalde
Microbial autoinducers: molecular structure and biological function

E. San Sebastian
Molecular modelization of antimetastatic drugs and drug targets

A. Zubia
Antimetastatic drugs: an example of synthesis based on theoretical design

X. Lopez
QM and QM/MM studies on phosphate diester hydrolysis reactions

F. Himo
DFT studies of radical enzymes

A. Rubio
Optical properties of biomolecules within TDDFT: excited state electron ion dynamics

M. Duran
A new vision of aromaticity through the electron-pair density

J. Llano
Thermochemistry of electron, proton, and proton-coupled electron transfer reactions in solution

D. York
Computational methods for RNA catalysis

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Workshop 2003

Physics meets Biology: Scattering and Computer Simulations

JUNE 25-28, 2003

Chairmen
Prof. J. Colmenero (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)
Prof. D. Richter (IFF Jülich, Germany)

The idea is to put together a reduced number of experts coming from different but related areas - scattering and computer simulation - in order to explore new routes, ideas and synergies for the future of this field.

CONTRIBUTIONS

D. Richter	**Neutron scattering in soft condensed matter**
J. Colmenero	**Doing MD simulation in polymers as a neutron scattering practitioner**
SELF ASSEMBLY	
A.R. Khokhlov	**Biomimetic sequence design and evolution of sequences in copolymers**
A. Semenov	**Hierarchical structure, fibrils and globules in heteropolymer systems**
PROTEIN DYNAMICS	
F. Parak	**The dynamics of proteins with characteristic times from femtoseconds to microseconds**
PROTEIN DYNAMICS - NEUTRON SCATTERING AND MODELLING	
J. Smith	**Protein dynamics and hydration: Scattering meets computer simulation**
M.C. Belissent-Funel	**Internal motions in proteins: a combined neutron scattering molecular modelling approach**
THE INFLUENCE OF SOLVENTS	
D. Tobias	**Hydration effects**
A. Sokolov	**Influence of solvents on the dynamics of proteins and DNA**
PROTEIN FOLDING	
T. McLeish	**Protein folding down to (hyper-)gutter?**
A. Grosberg	**Title to be announced**
MEMBRANES	
G. Gompper	**Budding of crystalline domains in fluid membranes**
D. Roux	**DNA in multilamellar vesicles – a new vector for drug delivery**

MEMBRANES AND MOLECULAR MACHINES

F. Goñi **Cell membranes: a few questions for physicists**

P. Timmins **The role of troponin in the regulation of vertebrate muscles**

Round table discussion
Future perspectives of a joined neutron scattering and simulation approach

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Workshop 2003

Optical Properties of Complex Materials over Different Length Scales

JULY 7-11, 2003

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Prof. F. Meseguer (Unidad Asociada CSIC-UPV, Valencia, Spain)
Prof. A. Modinos (National Technical University of Athens, Greece)
Prof. J. Pendry (Imperial College, London, UK)

The aim of this workshop is to bring together researchers with backgrounds in theory and experiments in order to assess the present state of our understanding of small particles as building blocks of meta-materials with engineered optical properties. This will cover the interaction of light with both photonic crystals and non-periodic structures at different wavelength scales ranging from the far infrared to the visible, as well as the theoretical and experimental techniques that are needed to investigate them. The main purpose is to combine knowledge about small particle characterization and complex systems of particles to gain insight and establish new links and future collaborations.

This workshop is of special interest to researchers conducting theoretical or experimental studies on:

Effective media and meta-materials

Optics from the nanometer to the millimeter scale

Collective excitations and plasmons

Photonic crystals

Electron diffraction: bridging the gap between electron and radiation waves

Electron microscopy

CONTRIBUTIONS

T. Ebbesen	**Diffraction control and enhanced transmission through sub-wavelength apertures in metal films**
L. Martín Moreno	**Extraordinary optical properties of nanostructured metals**
J. Prikulis	**Light scattering by small holes in thin metal films**
M. Sorolla	**Electromagnetic band gaps in planar microwave technology**
N.I. Zheludev	**Fundamental symmetries of light's interaction with planar chiral nanostructures**
M. Nieto-Vesperinas	**Electromagnetic forces in the near field**
T. Heinz	**Surface nonlinear optics of nanostructures**
E. Ozbay	**Physics and applications of 2D and 3D photonic crystals**
S. Tretyakov	**Physical means to store and amplify evanescent modes**
J. B. Pendry	**Designing lenses for the near field**
R. Marqués	**Amplification of evanescent waves and subwavelength focusing in feasible simple physical systems**
V. M. Shalaev	**Plasmonic nanoantennas for guiding light and sensing molecules**
S. Coyle	**Chameleon metals-metallic meshes from self-assembled colloids**
H. Benisty	**Planar photonic crystal: the example of InP-based phtonics and the relevant length scales in actual applications**
A. Modinos	**Photonic band gaps and disorder effects**
B. Barnes	**Surface plasmon length scales**
F. Meseguer	**New architectures in opal structures**
N. Zabala	**Electron energy loss analysis of nanoporous alumina films**
N. Yamamoto	**Light emission from nano-structures induced by high-energy electron beans**
A. Howie	**Where is spatially revolved spectroscopy going?**
C. Genet	**The Casimir force: theory-experiment comparison**
A. Dereux	**Oxides and metal nanostructures for controlling optical processes at the subwavelength scale**
C. N. Afonso	**Optical properties of nanostructured metal nanocomposites**
M. Käll	**Optical properties and applications of gold and silver nanoparticles**
J. Aizpurua	**Simulating nanoscale optical microscopy and spectroscopy**
L. Blanco	**Spontaneous emission in the presence of nanostructured materials**
D. Wiersma	**Complex dielectric systems with external control: from photonic crystal switching to tunable random Laser action**
A. Postigo	**Photonics crystals in active media: design and fabrication at the IMM**
L. Guidoni	**Femtosecond dynamics of light transmission through sub-wavelength hole arrays in metallich films**

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Donostia Encounters on Particle-solid Interactions

Modifications following different interaction processes at surfaces

SEPTEMBER 8-13, 2003

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The 5th Donostia Encounters on Particle-Solid Interactions was centered around the topic "Modifications following different interaction processes at surfaces". It was sponsored by the Donostia International Physics Center (DIPC). The chairman of the Conference, Prof. Archie Howi selected the following topics: photon and electron beam damage, charging effects in electron beam irradiation, environmental scanning electron microscopy, ion beam lithography and dry etching, computer simulation of condensed matter processes, ion and molecule scattering at surfaces and ion beam analysis.

CONTRIBUTIONS

MANIPULATION IN THE ATOMIC SCALE

N. Tolk
Desorption and damage studies at semiconductor surfaces and interfaces using intense, tunable, ultrafastlasers

J.I. Pascual
Mode-selective manipulation of the cleaveage of a single molecular bond

PHOTOCHEMISTRY AND LOW ENERGY ELECTRONS

D. Menzel
Photochemistry in adsorbates:Coupling-induced modifications, quenching, and selectivity

P. Rowntree
Interaction of low energy electrons with soft molecular systems

ION BEAM ANALYSIS

P. Pussa
Ion scattering as a tool for material science

F. Paszti
Interaction of MeV ions with porous materials: morphological changes and their investigation by ion beamanalysis

IONS AND ELECTRONS WITH INSULATORS

J. Cazaux
Electron irradiated insulators: mechanisms of charging and correlation with some chemical modifications

B. Thiel
Control of secondary electron emission from insulating surfaces by soft-landing ions in the low vacuum SEM

SMALL STRUCTURES

P. Kruit
Electron-beam-induced deposition of sub-10 nanometer structures

J.R. Sabin
Ion Induced Molecular Fragmentation

ENERGY LOSS AND ELECTRON EMISSION

V.A. Khodyrev
The current density approach in treatment of energy loss

M.S. Gravielle
Differential electron emission spectra produced by grazing ion-surface collisions

ION-SURFACE INTERACTIONS

P. Bauer
Electronic interactions of slow He ions at a metal surface

D. Boerma
Surface and thin layer physics at the CNAM of the UAM

TECHNOLOGICAL APPLICATIONS

J. Colligon
Modification of surface hardness using ion-assisted deposition

W.H. Bruenge
Ion projection direct structuring of surfaces: technology and applications

MOLECULES AT SURFACES

D. Farias
Looking at the hydrogen dissociation process via diffraction experiments

F. Busnengo
Low energy H2 scattering from metal surfaces: reactivity and dissociation mechanisms

ELECTRONS AND PHOTONS IN CRYSTALS

N. Vast
Anisotropy of the microscopic fluctuations of the polarization, confinement effects, and the dielectric function of crystals

F.J. G. de Abajo
The Cherenkov effect in photonic crystals

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Workshop 2003

Theoretical Biophysics Symposium

SEPTEMBER 21-24, 2003

Chairmen
Prof. R.W. Godby (York University, UK)
Prof. A. Rubio (Univesidad del País Vasco, Euskal Herriko Unibertsitatea, Spain)

Organizers
Dr. P. García-González (Universidad Autónoma de Madrid, Spain)
Prof. A. Rubio (Universidad del País Vasco, Euskal Herriko Unibertsitatea, Spain)

The aim of this workshop is to assess the present status of theoretical approaches to the study of spectroscopic properties of real materials, and explore their capability for applications in further systems with technological and biological interest. Due to the different methods used to tackle this problem (Many-Body Theory, Density Functional Theory, Configuration Interaction, semi-empirical approaches), this workshop is intended as a way to promote links among scientists coming from different communities working or interested in electron excited states.

CONTRIBUTIONS

THEORETICAL FOUNDATIONS I

E.K.Gross
ELFs and Ghosts in Density FunctionalTheory

Y.M. Niquet
High-accuracy XC potentials from the linear-response Sham-Schluter equation: Asymptotic behavior and properties

THEORETICAL FOUNDATIONS II

F. Sottile
Parameter-free calculation of response functions in time-dependent density-functional theory

A. Marini
Bound excitons in time-dependent density-functional-theory: optical and energy-loss spectra

S. Biermann
Electronic structure of strongly correlated materials-a view from dynamical mean field theory

BIOLOGICAL AND ORGANIC SYSTEMS I

P. Carloni and M. Rohlfing
Dynamics of electronically excited molecules

COMPLEX SYSTEMS I

G. Onida

Calculating optical spectra of surfaces and other non infinite systems using plane waves in DFT-LDA and Beyond: bottlenecks and progresses

O. Gunnarsson

Calculation of dynamical correlation functions: Application to resistivity saturation

COMPLEX SYSTEMS II

C. Hogan

Electron energy loss spectroscopy at As-rich GaAs(001) surfaces

M. Friak

Ab Initio investigation of the Halfmetal-Metal transition in magnetite

K. Tsemekhman

Self-Consistent Self-Interaction corrected DFT: The Method and applications to extend and confined systems

K. Tatarczyk

Surface plasmons in surface alloys

BIOLOGICAL AND ORGANIC SYSTEMS II

F.J. Himpsel

Electronic excitations at the interface between soft and hard matter

G. Schmidt

Ground-and excited-state properties of small molecular systems: Pyrimidine and purine bases in the gas phase and adsorbed on silicon

BIOLOGICAL AND ORGANIC SYSTEMS IV

A. Seitsonen

TDDFT in molecules and extended systems

A. Castro

BIOLOGICAL AND ORGANIC SYSTEMS V

M. Sulpizi

A Hybrid time-dependent density functional/molecular mechanics investigation of aminocoumarins in solution

E. Molinari

Optics and transport of (bio) molecular systems: solid state effects and P-P interactions

A. Calzolari

Electron channels in biomolecular nanowires

G. Stefanucci

Different ways of treating the bias and the inclusion of many-body interactions in the description of quantum conductance

ELECTRON TRANSPORT

J. G. Herrero

Measuring the electrical transport properties of individual molecules: carbon nanotubes and DNA

P. Bokes

Coherent steady current-carrying states from the maximum entropy principle and the Kubo Formula

A. Wacker

Nonequilibrium quantum transport in quantum cascade lasers

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PUBLIC LECTURES

DIPC hosts a number of events promoting social awareness of science and the wider implications of scientific activity.

Public Lecture

Science and Its Frontiers

NOVEMBER 13-14, 2003

Program Committee
Prof. P. M. Echenique (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)
Prof. J. J. Iruín (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)
Prof. I. Tellería (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)
Prof. J. J. del Val (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)

Science, in its different areas, has a great importance in today's culture, not only from an economic and strategic point of view but also in the advancement of nature's knowledge. Teacher's of Secondary Education play an important part in transmitting scientific concepts and values to the youngest generations. We organize these lectures on "Science and its frontiers" to help teachers in their daily task, showing them the latest advances in Physics, Chemistry, Biology and Medicine. Speakers are internationally known researchers. These lectures have been included in Basque Government's Education Council's GARATU program.

PARTICIPANTS

There were 140 participants that came from diverse disciplines:
· 20 university teachers
· 60 Highest Formative Cycles and Secondary Education teachers
· Researchers
· Fellows
· Experts in varied areas of science
· Others interested in scientific activity

CONTRIBUTING LECTURES

J. Rodés
Research in Biomedicine
In this talk, the evolution of medical care since the beginning of the 20th century is explained through the changes observed in a reference center such as Hospital Clínico in Barcelona. The needs of this type of center are justified, including a strong research unit driven to provide fast and effective responses to changing sanitary requirements.

J. M. Pitarke
Powers of ten. On the size of components on the Universe
Powers of ten are used to discuss the relative size of the components of the Universe, from the inside of a proton to the farthest reaches of the Universe. The fundamentals of matter and force are discussed, as well as the history and fate of the Universe.

J. Colmenero

The world of "Soft Condensed Materia"

The concept of "soft matter" subsumes a large class of molecular materials, including e.g. polymers, thermotropic liquid crystals, micellar solutions, microemulsions and colloidal suspensions, and also includes biological materials, e.g. membranes and vesicles. These substances have a wide range of applications such as structural and packaging materials, foams and adhesives, detergents and cosmetics, paint, food additives, lubricants and fuel additives, rubber in tires etc., and our daily life would be unimaginable without them. In spite of the various forms of these materials, many of their very different properties have common physicochemical origins. The structural units of soft matter systems are large molecules or aggregates of molecules showing different structural and dynamical properties depending on the length scale of observation. The main goal of this talk is to give a general introduction to this class of important materials, including a historical perspective of the scientific development of this rather new field.

H. Ostolaza

The basis of life

Since the experiment of S. Miller and H. Urey , in 1953, where small inorganic molecules yielded organic compounds including amino acids, a new understanding of the workings of RNA and DNA, the building blocks of life, have emerged. The recent discovery of prebiotic conditions on other planets and the announcement of a bacterial fossil originating on Mars has brought new attention to the study of life's origins.

G. Morata

DNA. First 50 years

The discovery of the structure of DNA is one of the most important scientific findings of the 20th century and one that has shaped biological research during the last 50 years. Two basic problems of Biology, the nature and the replication of the genetic information, were solved at once by the discovery of the DNA double helix. The realization that the genetic information is encoded in the lineal arrangement of the four bases (A)denine, (T)imine, (C)itosine and (G)uanine, that form the backbone of DNA, changed completely the approach of experimental biology. The focus in the study of the intimate structure and properties of DNA has resulted in a profound insight as to the basic mechanisms of life. It has also made possible the development of extraordinarily powerful methods to manipulate the genetic information. These methods already have applications of social and economical interest in the improvement of live stocks and cultivated plants. They are also potentially very important in Biomedicine as they offer the possibility of new and revolutionary treatments for genetic and degenerative diseases.

M.A. Peña

Hydrogen fuel cells. Future Power

Fuel Cells and Hydrogen are words that go together when someone wants to talk about the future of energy: Fuel Cells as high efficiency systems, and Hydrogen as its most suitable environmentally friendly fuel. But a lot of scientific and technological work is still required. The developing of new technology for the mass production of Fuel Cells, and the implementation of the Hydrogen economy, from the fossil feedstock to renewable sources, will be the driving force of the energy world during the next years.

E. Ortega

Nanotechnology: At the frontiers of the Atom

Nanotechnology, or the technology made at the atomic scale is becoming a reality. In order to accommodate to the nanotechnology era, the microlectronics industry will undergo a thorough conceptual transformation, a revolution. The reason is that the behavior of the matter completely changes at the atomic scale, which is governed by quantum mechanics. In this lecture we will review the fundamental limits of current technologies when scaling down to the atomic limit, as well as the more exciting perspectives of nanotechnology.

F. Cossio

XXI Century's Chemistry: Molecular and supramolecular worlds

In this lecture a concise analysis of the origins and present situation of chemistry was presented, as well as the perspectives of chemical sciences for the XXIth century, both in the scientific and social contexts. The main topics discussed concerned the impact of chemical problems on what remains to be discovered. As outstanding examples, the problem of chemical synthesis of high-value molecules such as taxol and the productivity gap of pharmaceutical industry were presented. Finally, the main aspects of information storage and transmission using the concepts and tools provided by supramolecular chemistry were briefly discussed.

J. Marcaide

Young universe

The expansion of the Universe and the cosmic microwave background (CMB) suggest a singular episode about 14 billion years ago, a leviathan explosion dubbed the Big Bang, with extremely high temperatures and densities. A new cosmology has arisen from the combined efforts of physicists and astronomers. The acoustic peaks in the CMB angular spectrum and the large-scale power spectrum have provided rich information on the cosmological parameters. A wealth of data on the apparent brightness of type Ia supernova favor an accelerating Universe, and mysterious attractive dark matter and repulsive dark energy seem to dominate the matter/energy budget.

M. Delibes

How did Nature's preservation develop to Biology

Human concern in the face of Nature's deterioration probably dates back several thousand years. Plato was attributed the comparison of the barren mountains of Attica with the "bare bones of a consumed body". Throughout the 18th century, arguments accumulated postulating an undesirable influence of human activity on the natural wealth, which clashed with the idea that our species was little less than the administrator of God's designs. The tight connection between the interest to know the environment and the concern for conservation, which gave rise to conservation biology started in the 19th century, supported by the evidence that all living beings occupy a finite world (eg. Humboldt) and shared a phylogenetic history (Darwin). Two different approaches tied to conservation and protection have emerged since 1980 called conservation biology, which has combined modern population ecology with traditional disciplines which in turn are separated from each other. Perhaps the most innovating of conservation biology has been to integrate conservationist theory and practice, dispersed under the cover of the neodarwinist paradigm. That achievement has converted old conservation into biology, as Dobzhansky would say: "nothing in biology makes sense outside the light of evolution". The evolutionist framework affects traditional conservationist arguments, as we have sketched out.