OUR RESEARCHERS

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

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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).