

# OUR RESEARCHERS

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

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## FELLOWS GIPUZKOA

### DR. A. MORENO

University of Roma La Sapienza, Italy  
01-01-2005

Investigation by means of molecular dynamics and Monte Carlo simulations of:

- Energy landscape and non-ergodic transitions in supercooled liquids
- Dynamics of linear molecules in disordered static environments
- Dynamic heterogeneities in polymer blends

### DR. V. SILKIN

Russian Academy of Science, Tomsk, Russia  
03-01-2002

- Surface science
- Electronic excitations at the metal surfaces
- Electron dynamics in metals, metal surfaces and systems with reduced dimensionality

### DR. M.A. CAZALILLA

ICTP Trieste, Italy  
01-01-2003

- Strongly correlated systems, Bose Condensates, Mesoscopic and low-dimensional systems in and out of equilibrium
- Electronic excitations in surfaces and anisotropic systems

### DR. M. ALDUCIN

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain  
01-09-2003

- Lifetime of low energy electrons in paramagnetic materials: spin effects and non-linear effects
- Interaction of atoms/ions with surfaces: charge exchange and energy loss
- Dielectric response of covered metal surfaces

### DR. J. AIZPURUA IRIAZABAL

National Institute of Standards and Technology (NIST), USA  
01-01-2004

Electronic and optical properties of metal nanostructures and semiconductor low-dimensional systems.

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

## WHAT IS FELLOWS GIPUZKOA ?

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

## POST-DOCTORAL POSITIONS

### DR. J. SACRISTÁN

Instituto de Ciencia y Tecnología de Polímeros, CSIC, Madrid, Spain  
01-04-2002 through 31-03-2005

My research focuses on the application molecular dynamics methods to study the structure and properties of a variety of polymer on the atomic scale. We are interested in bulk, free and confined polymer systems, glass transition in polymer films, static and dynamic properties of thin polymer films.

### DR. A. AYUELA

Helsinki Technical University, Finland  
14-05-2003

- Ab-initio studies of magnetism with dimensionality (magnetic anisotropy, spin spirals, Curie temperature...): nanowires, multilayers, magnetic shape memory alloys
- Phase field and ising description of magnetic phenomena

### DR. F. SCHILLER

Universität Dresden, Germany  
01-10-2003 through 31-08-2005

Crystalline and electronic structure of thin Be and Mg films.

### DR. M. GRÜNING

Vrije Universiteit, Amsterdam, The Netherlands  
15-11-2003 through 31-12-2005

Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

### DR. C. CORRIOL

University of Liverpool, UK  
01-01-2004 through 31-12-2005

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

### DR. I. NECHAEV

Statal University of Tomsk, Russia  
10-02-2004

Electron excitations in ferromagnetic materials.

### DR. S. CERVENY

Chalmers University of Technology, Sweden  
01-03-2004

General framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other experimental techniques and MD-simulations.

### DR. G. SCHWARTZ

Chalmers University of Technology, Sweden  
01-03-2004

General framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other experimental techniques and MD-simulations.

### DR. D. CANGIALOSI

University of Delft, Holland  
01-03-2004

Positron annihilation lifetime spectroscopy to study the dynamics of polycarbonate far below  $T_g$ .

### DR. M. TYAGI

Jawaharlal Nehru University, India  
04-03-2004

The general framework of dynamic properties of glass forming polymers by dielectric spectroscopy in combination with other techniques as, for instance, quasielastic neutron scattering and MD-simulations as well.

### DR. R. GÓMEZ-MEDINA

Universidad Autónoma de Madrid, Spain  
27-09-2004 through 31-12-2005

Calculate photon emission probabilities upon electron bombardment in various metallic nanostructures. This will be compared with recent experimental results from Prof. N. Yamamoto in order to develop a systematics to map plasmon-mode spatial distributions in complex geometries by means of light emission measurements using scanning transmission electron microscopes.

### DR. R. GAUDOIN

Rutgers University, New Jersey, USA  
15-11-2004

An important issue in many-body and density-functional theory is to understand not only whether the LDA works for a strongly inhomogeneous electron gas, but also to understand whether the nonlocal xc kernel  $f_{xc}$  of an inhomogeneous electron gas can be built from the corresponding nonlocal xc kernel  $f_{xc}$  of a homogeneous electron gas, a question which was raised by Kohn and Krotscheck many years ago [Phys. Rev. Lett. 57, 862 (1986)] but which has not been solved so far. In order to investigate this issue, we plan to

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

**DR. A.C. GENIX**

Laboratoire de Recherche sur les Polymères, Thiais Université Paris XII, France  
01-12-2004

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

**DR. S. ARRESE-IGOR**

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain  
01-01 through 06-04-2005

Sub-Tg molecular motions in engineering thermoplastics.

**DR. M.J. CABRERA SAN FÉLIX**

University of Liverpool, United Kingdom  
01-04-2005

Molecular Modelling of water ice in atmospheric and astrophysical environments.

## TEMPORARY CONTRACT POSITIONS

**DR. V. ZHUKOV**

Ural Branch of Russian Academy of Sciences, Ekaterunbourg, Russia  
01-11-2005

Basing on the LMTO band-structure approach, was developed a first-principle GW+T method of the excited electrons lifetimes calculations. Method combines the evaluation of the lowest term of self-energy within GW approach with the calculations of the highest terms within T-matrix approach. The method has been applied to analyze experimental data for Fe and Ni.

The role of non-spin-flip contributions, Stoner and magnon contribution to the lifetimes and line-widths of excited electrons have been evaluated.

**DR. I. SKLYADNEVA**

Russian Academy of Sciences, Tomsk, Russia  
14-05-2003 through 14-05-2006

Surface phonons and electron-phonon interactions in bulk metals and at metal surfaces. Electron-phonon interactions are of paramount importance for the correct description of the temperature dependence of quasiparticle dynamics in bulk metals and at metals surfaces. The goal of the present project is calculations of electron-phonon interactions for overlayers of alkali metals on simple and noble metal surfaces. These calculations will be also done for superconducting materials like MgB2 and for semimetals.

## PHD FELLOWSHIPS

### R. VINCENT

Université Paul Sabatier, Toulouse, France

01-11-2003

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

### R. PÉREZ APARICIO

Universidad de Valladolid, Spain

15-11-2003 through 31-08-2005

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

### I. ROMERO PÉREZ

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01-12-2003 through 31-08-2005

From a theoretical point of view, the electromagnetic response of different metamaterials formed by a periodic distribution of complex objects whose size is much smaller than the wavelength under consideration. These materials will behave like homogeneous media that will be described by their effective dielectric function and magnetic permeability. In particular, left-handed media belong to this class of materials. The main purpose of this work is to extract rules on how to construct metamaterials with on-demand optical properties, and in particular, artificial media that can sustain electric and magnetic resonances over a wide range of wavelengths.

### M. MARTÍNEZ CANALES

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01-10-2004 through 30-09-2005

Metallization and superconducting properties of hydrogen rich alloys at high pressure.

### I. IRADI LEICEAGA

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01-11-2004

Study of polystyrene: Molecular dynamics simulations and neutron scattering.

### M. MASSOT PÉREZ

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01-12-2004 through 15-05-2005

Electron energy loss spectroscopy and electronic excitations in nanostructures.

### A. SARASOLA IÑÍGUEZ

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01-12-2004 through 31-10-2005

Local density approximation in the study of energy loss problems in ion/atom and ion/surface problems.

### O. MICHELENA GONZÁLEZ

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01-01 through 31-05-2005

Study of the effects of thermo-mechanical treatments on Dielectric Secondary Relaxations of engineering thermoplastics.

### D. FERNÁNDEZ PÉREZ

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01-01 through 31-07-2005

Methyl group dynamics in disordered systems: Polysulfone, Polycarbonate, Phenoxy and PMMA; a 2H-NMR study.

### I. QUINTANA FERNÁNDEZ

Universidad de Cantabria, Spain

01-01-2005

The aim of the work is to find the relation between the molecular motions and the transport properties in a polymer membrane. By means of quasielastic neutron scattering, we study the molecular dynamics in a polymer membrane: polyethersulfone.

### S. CAPPONI

University of Perugia, Italy

23-10-2005

Dynamics of DNA and proteins by neutron scattering.