OUR RESEARCHERS

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

Fellows Gipuzkoa

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

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

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

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

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

What is Fellows Gipuzkoa?

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

Post-doctoral Positions

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

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

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

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

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

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

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

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

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

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

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

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

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

Dr. A.C. Genix

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

Dr. S. Arrese-Igor

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

Dr. M.J. Cabrera San Félix

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

Temporary Contract Positions

Dr. V. Zhukov

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

Dr. I. Sklyadneva

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

PhD Fellowships

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

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

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

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

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

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

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

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

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

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

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