



Strength

Researchers

Fellows Gipuzkoa

Dr. Angel Moreno Segurado

Sapienza Università di Roma, Italy

01/01/2005–26/06/2007

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. Vyacheslav Silkin

Russian Academy of Science, Tomsk, Russia

03/01/2002–15/12/2007

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

Dr. Miguel Angel Cazalilla Gutierrez

International Centre for Theoretical Physics, Italy

01/01/2003–07/06/2007

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

Dr. Maite Alducin Ochoa

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01/09/2003–28/06/2007

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. Javier Aizpurua Iriazabal

National Institute of Standards and Technology, Maryland, USA

01/01/2004

Electronic and optical properties of metal nanostructures and semiconductor low-dimensional systems. Nanooptics for field-enhanced microscopies and spectroscopies.

Dr. Arantazu García Lekue

Lawrence Berkeley National Laboratory, California, USA

01/10/2006

Electron transport and dynamics in nanostructure materials. Elastic quantum transport through molecular nanodevices, such as molecular based electronic switches. Inelastic effects caused by electronvibration interactions.

Dr. Asier Eiguren Goienetxea

Montanuniversität Leoben, Austria

11/06/2007

Study of the electron-phonon interaction in strongly correlated and strong coupling systems. Calculation of electron-phonon sensitive thermodynamic properties including, heat capacity, different susceptibilities and charge and spin transport in low dimensional systems. Implementation of the Wilson's Numerical Renormalization Group method to electron-phonon interaction. Comparative study of the limitations of the perturbative approaches in relation to the Renormalization Group. Superconductivity.

Dr. María José Cabrera San Félix

University of Liverpool, UK and Donostia International Physics Center, Spain

01/11/2007

Molecular Modeling of water ice in atmospheric and astrophysical environments.

Postdoctoral Positions

Dr. Andrés Ayuela

Helsinki University of Technology, Finland

14/05/2003–13/07/2006

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

Dr. Ilya Nechaev

Tomsk State University, Russia

10/02/2004–31/01/2007

Electron excitations in ferromagnetic materials.

Dr. Silvana Cerveny Murcia

Chalmers University of Technology, Sweden

01/05/2004–28/02/2007

Dynamic properties of water in glass forming polymers and biological systems by dielectric spectroscopy in combination with neutron scattering.

Dr. Gustavo Schwartz

Chalmers University of Technology, Sweden

08/06/2004–28/02/2007

Dynamic properties of glass forming polymers by dielectric spectroscopy under hydrostatic pressure in combination with other experimental techniques.

Dr. Daniele Cangialosi

Technische Universiteit Delft, The Netherlands

01/03/2004–28/02/2007

Models for dynamics of miscible polymer blends.

Dr. Madhusudan Tyagi

Jawaharlal Nehru University, India

04/03/2004–30/04/2007

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. René Gaudoin

Rutgers University, New Jersey, USA

15/11/2004–31/07/2006

Diffusion Monte Carlo investigations of electron correlation in bulk systems and solid surfaces.

Dr. Anne Caroline Genix

Laboratoire de Recherche sur les Polymères, Université Paris XII, France

01/12/2004–31/08/2006

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. María José Cabrera San Félix

University of Liverpool, United Kingdom

01/04/2005–31/10/2007

Molecular Modeling of water ice in atmospheric and astrophysical environments.

Dr. Reidar Lund

IFF-FZ, Forschungszentrum Jülich, Germany

20/02/2006

Dynamics in functionalized polymers

Dr. Tatiana Teperik

Russian Academy of Sciences, Saratov, Russia

03/06/2006–31/10/2007

Electromagnetic optics. Collective resonances in nanostructures.

Dr. Lucian Constantin

Tulane University, Louisiana, USA

01/10/2006–15/09/2007

Many-body exchange-correlation effects at metal surfaces.

Dr. Antonios Balassis

City University of New York, USA

13/11/2006–30/09/2007

Collective electronic excitations in systems of reduced dimensionality.

Dr. Iñaki Silanes Cristóbal

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01/01/2007

Surface-assisted assembly of two dimensional molecular networks with different coordination symmetry. Study of oxygen adsorption on several Porphyrins (Fe and Mg coordinated). Molecular Switches based on different conformational change induced architectures.

Dr. Martina Corso

Universität Zürich, Switzerland

02/01/2007

Boron nitride nanomesh: a peculiar self-assembled nanostructure.

Dr. Gisela Bocan

Universidad de Buenos Aires, Argentina

01/02/2007

Gas/surface dynamics.

Dr. Thomas Frederiksen

Danmarks Tekniske Universitet, Denmark

01/05/2007

First-principles modeling of elastic and inelastic transport in nanoscale junctions.

Dr. Daniel Bozi

Instituto de Ciencia de Materiales-CSIC, Madrid, Spain

01/08/2007

Study of the properties of the low-dimensional systems that can be realized by loading ultra cold atomic gases in optical lattices or other types of very anisotropic traps. Study of the absence of thermalization in integrable realizations thereof. Calculation of correlation properties in strongly interacting systems. Study of the atom-surface interactions, the Casimir Effect in and out of equilibrium.

Dr. Alejandro Reyes Coronado

Universidad Nacional Autónoma de México, México

30/08/2007

Optical response of resonant metallic nanostructures in surface-enhanced microscopy and spectroscopy.

Dr. Dimas Garcia de Oteyza Feldermann

Max-Planck-Institut, Stuttgart, Germany

01/09/2007

The scientific work will be focused on the development of atomic force microscopy instrumentation for dielectric and conductivity measurements, in particular in polymers and semiconducting oligomers. The work will be further complemented by absorption and photoemission experiments.

Dr. Emil Lezak

Polish Academy of Sciences, Lodz, Poland

02/09/2007

Plastic deformation of gamma phase isotactic polypropilene in the plane-strain compression.

Dr. Dusan Racko

Slovak Academy of Sciences-Polymer Institut, Bratislava, Slovak Republic

03/09/2007

Molecular dynamics simulations in polymers.

Dr. Mario Piris Silvera

Universität Erlangen-Nürnberg, Germany

01/10/2007

Natural Orbital Functional Theory (NOFT). Correlation studies by means of electron-pair density functions. Description of van der Waals interactions. Characterization of ZnS nanostructures endohedrally doped with transition metals. Study of ZnS, BN and SnI₂ nanoclusters and solids.

Dr. Nikolay Zaytsev

Siberian Institute of Physics and Technology, Tomsk, Russia

04/10/2007

Study of spin dependent electronic structure and spin-orbit interaction at clean metal surfaces and at surfaces with adsorbate. This activity has attracted much attention last years both experimentally and theoretically. The study of electronic structure of carbon surface as well as of noble metal and ferromagnetic metal surfaces.

Temporary Contract Positions

Dr. Irina Sklyadneva

Russian Academy of Sciences, Tomsk, Russia

14/05/2003

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.

Dr. Vladlen Zhukov

Russian Academy of Sciences (Ural Branch), Yekaterinburg, Russia

01/11/2005–28/12/2007

Based 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. Alvaro Rodriguez Prieto

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01/11–31/12/2007

Electronic properties of light alkali metals under high pressure. The simple behavior alkaline metals present at normal conditions breaks when high pressures applied. One of the most important features telling about the pressure induced complexity in Li and other alkali metals is the drastic increase of its superconducting transition temperature, from 0.4 mK at equilibrium up to 14 K at P=30 GPa. I apply state of the art computational methods in order to understand the physical origin of this striking behavior.

Dr. Maia García Vergniory

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

05/12/2007

Many body and band structure effects on the interaction between hot electrons and ions with solid surfaces.

PhD Fellowships

Remi Vincent

Université Paul Sabatier, Toulouse III, France

01/11/2003

Ions induced electron excitations in ferromagnetic materials. Interaction of ions with metals energy loss and stopping power. Study of metallic clusters. Response function.

Itziar Iradi Leiceaga

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01/11/2004–12/11/2006

Study of polystyrene: Molecular dynamics simulations and neutron scattering.

Iban Quintana Fernandez

Universidad de Cantabria, Spain

01/01/2005–31/01/2007

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.

Sara Capponi

Università degli Studi di Perugia, Italy

03/10/2005

Dynamics of DNA and proteins by neutron scattering.

Aitzol Garcia Etxarri

Escuela Superior de Ingenieros, tecnun, Universidad de Navarra, Spain

01/04–30/09/2006

Electromagnetic interactions in nanoscale field enhanced microscopies and spectroscopies.

Iñigo Aldazabal Mensa

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01/07/2006

Electron emission in ion-surface grazing collisions; contributions to the convoy electrons. Wave packet propagation techniques applied to STM systems. Laser induced electron emission in metallic surfaces.

Maia García Vergniory

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01/07/2006–04/12/2007

Many body and band structure effects on the interaction between hot electrons and ions with solid surfaces.

Arturo Narros Gonzalez

Universidad de Salamanca, Spain

01/07/2006–31/12/2007

Studies of glass transition in polymers: molecular dynamics simulations and neutron scattering.

Elton José Gomes Santos

Universidade Federal do Ceará, Brasil

26/08–31/12/2006

Electronic structure calculations for the description of nanostructure materials with technological applications.

Martin Brodeck

IFF-FZ, Forschungszentrum Jülich, Germany

01/10/2006

Combined study by means of molecular dynamics simulations and neutron scattering measurements of the strongly decoupled dynamics which are exhibited by the different components of polyethyleneoxide/polymethylmetacrylate blends which can differ up to 12 orders of magnitude in local relaxation times.

Yon Sánchez Paisal

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

16/10/2006

Electronic structure calculations in nanostructured systems with technological applications.

Xabier Zubizarreta Iriarte

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

16/10/2006

Electronic structure and excitations in metals with strong spin-orbit interaction.

Asier Zugarramurdi Camino

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

02/11/2006–31/12/2007

Electronic structure and excitations in nanostructures. Quantum size effects of nanostructures supported on surfaces.

Olalla Pérez González

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

02/11/2006

Plasmon excitations in metallic nanoparticles. Optical properties of nanostructured materials.

Juan Pablo Echeverry Enciso

Universidad del Valle, Cali, Colombia

28/08/2007

Study of collective electronic excitations and dynamic of reduced symmetry systems.

Lourdes Del Valle Carrandi

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

03/09–31/12/2007

Microscopic (atomic and molecular) comprehension of the dynamic processes which take place in multi-component and nano-structured polymers.

Clément Riedel

Université Montpellier 2, France

05/09/2007

Multiscale study of the dielectrics properties of matter from the nanoscopic scale to the macroscopic scale.

Nicolas Large

Université Paul Sabatier, Toulouse, France

01/10/2007

Raman spectroscopy in low dimensional semiconductor structures.

Sandra Plaza García

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01/10/2007

Dynamics of functionalized polymers. Polymer functionalization is a promising tool for the development of future polymer applications. We want to know how functionalization modifies the matrix properties which is in connection with the technological application of functionalized polymers.

Ion Errea Lope

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

10/10–31/12/2007

The aim of this research is to perform a theoretical ab initio study of superconductivity and other anomalies in simple materials under pressure. For instance, we will focus on the electron-phonon interaction, response function and other properties that will help us to characterize the complexity induced by pressure on this materials.

Marco Bernabei

Università degli Studi Roma Tre, Italy

29/10/2007

Molecular dynamics simulations of simple models for glass-forming polymers.

Marina Quijada Van den Berghe

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

01/11/2007

Electron dynamics in metal clusters. Study of the size effects in the lifetime of excited electrons in metal clusters. TDDFT calculation of the energy loss in collision processes of charges with metal clusters.

Itziar Goikoetxea Martinez

Universidad Complutense de Madrid, Spain

01/12/2007

Non-adiabatic processes in the adsorption of diatomic molecules on metal surfaces.

Eneko Malatsetxebarria Elizegi

Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain

31/12/2007

Low dimensional quantum many-body systems.