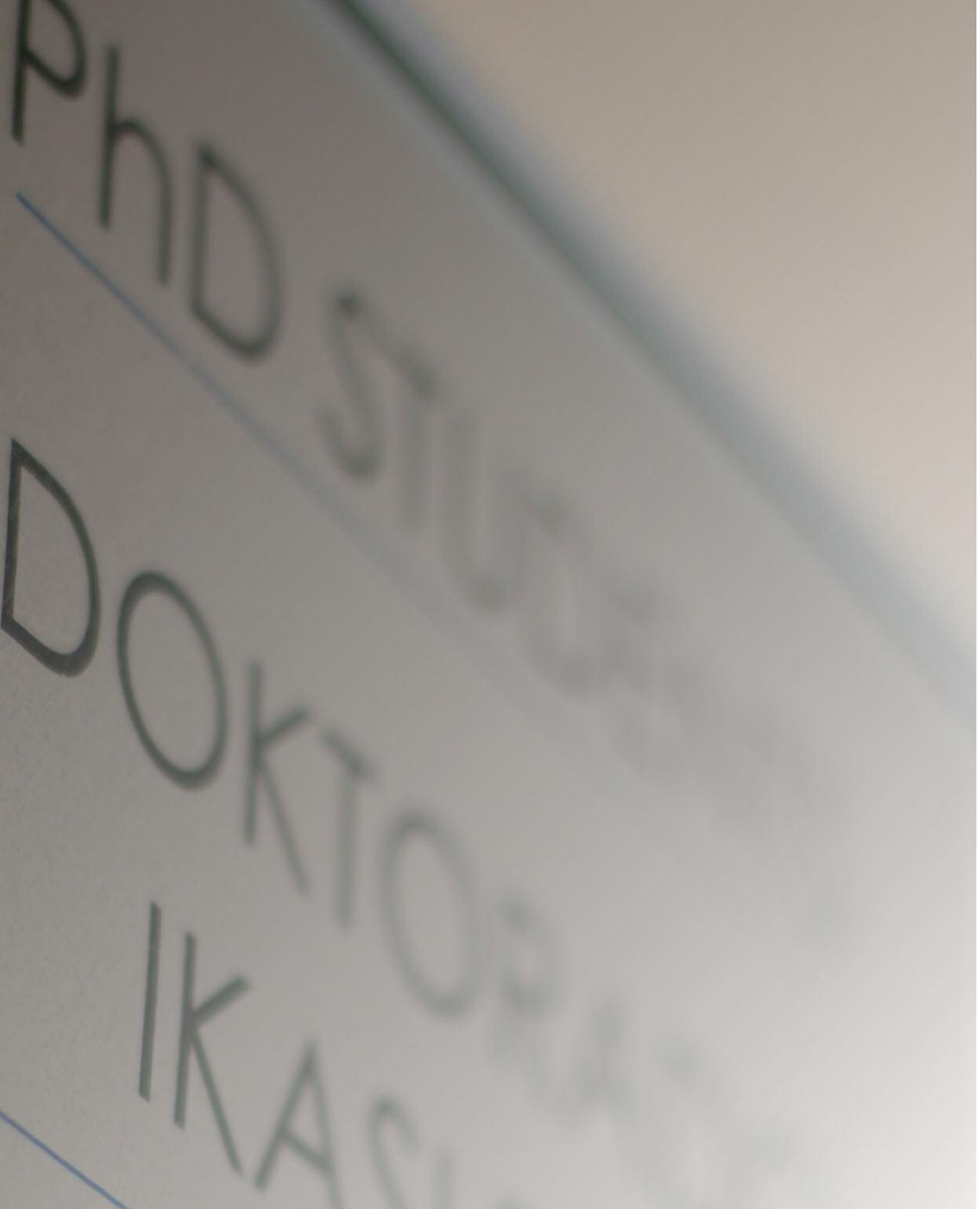

Researchers

Fellows Gipuzkoa

Dr. Javier Aizpurua Iriazabal
National Institute of Standards and Technology, USA
01/01/2004–31/07/2008
Electronic and optical properties of metal nanostructures and semiconductor low-dimensional systems. Nanooptics for field-enhanced microscopies and spectroscopies.

Dr. Arantzazu Garcia Lekue
Lawrence Berkeley National Laboratory, USA
01/10/2006–Present
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
University of Leoben, Austria
11/06/2007–05/10/2009
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, United Kingdom and Donostia International Physics Center, Spain
01/11/2007–Present
Molecular modelling of water ice in atmospheric and astrophysical environments. First-principles calculations of the structural properties and reactivity of water adsorbed, at the monolayer and submonolayer regions, on different surface types: metallic, ionic and graphitic surfaces.

Dr. Thomas Frederiksen
Technical University of Denmark
01/03/2008–Present
Theory and simulation of electronic transport properties of nanoscale systems. First-principles modeling of current-induced phenomena, inelastic scattering, and local heating. Density functional theory, non-equilibrium Green's functions, electron-phonon coupling, molecular electronics, monatomic chains, fullerenes.

Dr. Laura Férnandez Gómez-Recuero
Technische Universität Dresden, Germany
01/01/2009–Present
Preparation and characterization of self-assembled metallic nanostructures that reveal magnetic properties. Structural analysis by scanning tunneling microscopy. Magnetic characterization by magnetometry and magneto-optics.

Postdoctoral Positions

Dr. Reidar Lund
IFF-FZ, Forschungszentrum Jülich, Germany
20/02/2006–Present
Dynamics in funcionalized polymers.

Dr. Iñaki Silanes Cristóbal
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/01/2007–15/03/2008
Surface-assisted assembly of two dimensional molecular networks with different coordination symmetry. Study of oxygen adsorption on several Pophyrins (Fe and Mg coordinated). Molecular Switches based on different conformational change induced architectures.

Dr. Martina Corso
University of Zurich, Switzerland
02/01/2007–16/10/2009
Boron nitride nanomesh: a peculiar self-assembled nanostructure.

Dr. Gisela Bocan
Universidad de Buenos Aires, Argentina
01/02/2007–07/02/2009
Gas-surface systems. Dynamics of diatomic molecules impinging on metallic surfaces. Dissociative adsorption and Scattering. Exchange-correlation and DFT calculations. Potential Energy Surface Calculations.

Dr. Thomas Frederiksen
Technical University of Denmark
01/05/2007–29/02/2008
Theory and simulation of electronic transport properties of nanoscale systems. First-principles modeling of current-induced phenomena, inelastic scattering, and local heating. Density functional theory, nonequilibrium Green's functions, electron-phonon coupling, molecular electronics, monatomic chains, fullerenes.

Dr. Daniel Bozi
ICMM, CSIC, Madrid, Spain
01/08/2007–18/12/2008
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 corrlation 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
30/08/2007–31/08/2009
Optical response of resonant metallic nanostructures in surface-enhanced microscopy and spectroscopy.

Dr. Dimas Garcia de Oteyza Feldermann
Max Planck Institute for Metal Research, Stuttgart, Germany
01/09/2007–Present
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–Present
Plastic deformation of gamma phase isotactic polypropilene in the plane-strain compression.

Dr. Dusan Racko
Polymer Institut Slovak Academy of Sciences, Bratislava, Slovak Republic
03/09/2007–Present
Molecular dynamics simulations in polymers.

Dr. Mario Piris Silvera
University Erlangen-Nuremberg, Germany
01/10/2007–03/05/2008
Natural Orbital Functional Theory (NOFT). Correlation studies by means of electron-pair density functions. Description of van der Waals interactions. Characterization of ZnS nanostructures endohedraly doped with transition metals. Study of ZnS, BN and Sn12 nanoclusters and solids.

Dr. Nicolay Zaytsev
Sibirian Institute of Physics and Technology, Tomsk, Russia
04/10/2007–06/08/2009
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.

Dr. Maia García Vergniory
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
05/12/2007–31/01/2008
Many body and band structure effects on the interaction between hot electrons and ions with solid surfaces.

Dr. Claudio Horowitz
Centro Atómico Bariloche, Argentina
29/02/2008–28/02/2009
Optimized effective-potential approach to the Kohn-Sham exchange-correlation potential of density-functional theory.

Dr. Santiago Rigamonti
Centro Atómico Bariloche, Argentina
23/04/2008–Present
Electronic structure of low dimensional systems and transport in molecular junctions.

Dr. Marisa Faraggi
Universidad de Buenos Aires, Argentina
05/05/2008–Present
Dynamics of electronic excitation in metallic surfaces focusing on the study of electron-electron and electron-phonon interactions.

Dr. René Gaudoin
Rutgers University, New Jersey, USA
01/06/2008–20/02/2009
Diffusion Monte Carlo investigations of electron correlation in bulk systems and solid surfaces.

Dr. Virginie Boucher
University of Lille (ENSCL), France
30/10/2008–Present
Dynamical properties at molecular scale in polymeric materials multi-component and/or nano-structured, combining different experimental techniques and in particular, dielectric and mechanical spectroscopy. There is also the possibility of using also X-rays and neutron scattering.

Dr. Bruno Rousseau
Cornell University, USA
01/11/2008–15/05/2009
Theoretical analysis of pressure induced electronic and superconducting anomalies in simple elements and their alloys.

Dr. Remi Busselez
Universite de Rennes, France
03/11/2008–Present
The work will be focus on the study of dynamics at atomic and molecular scale in two-component polymeric systems with dynamic asymmetry by quasielastic neutron scattering and fully atomistic molecular dynamics simulations.

Dr. Vito Despoja
University of Zagreb, Croatia
22/02–15/05/2009
Within the present project will be investigated within framework of ab initio time-dependent density-functional theory the properties of excited electrons and holes and collective electronic excitations at the low-energy domain in iron-based metallic systems called pnictides which have been discovered recently and characterized by an elevated critical temperature of the superconducting transition.

Dr. Ludovic Martin
Université Bordeaux1, Talence, France
01/09/2009–Present
Theory of elementary reactive processes at metal surfaces: Calculation of potential energy surfaces from first-principles and evaluation of reaction rates in Eley-Rideal processes.

Dr. Lokendra Pratap Singh
School of Physical Sciences, Jawaharlal Nehru University, New Delhi, India
07/09/2009–Present
Extend the dielectric investigation on the dynamics of the systems in higher frequencies and to compare the results with those obtained by other techniques accessing the same frequency range, namely neutron scattering and molecular dynamic simulations.

Dr. Siddhart Surajbhan Gautam
Bhabha Atomic Research Centre, Mumbai, India
04/09/2009–Present
Structure and dynamics of polymers by neutron scattering and md-simulations.

Dr. Manfred Matena
University of Basel, Switzerland
01/11/2009–Present
Angle-resolved photoemission spectroscopy as well as scanning tunneling microscopy (STM) and spectroscopy (STS) are intended to be used for experimental studies on electronic and structural properties of molecular surface assemblies.

Temporary Contract Positions

Dr. Irina Sklyadneva
Russian Academy of Sciences, Tomsk, Russia
14/05/2003–Present
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. Andrey Kazanskiy
University of Saint Petersburg, Russia
17/07/2009–Present
Electron dynamics at adsorbates on metals. Study of electron ejection from different bands of metal by attosecond pulses has been continued. Ionization of an alkali atom adsorbed on a metal surface by attosecond pulse within a streaking scheme has been considered. A computational code for study Auger ionization by attosecond pulse within the streaking scheme has been developed. A study of interaction of an electron ionized from an inner shell of an adsorbed atom with its dynamically formed image charge is in progress.

Dr. José Alfonso Pomposo Alonso
CIDETEC, San Sebastian, Spain
16/11/2009–Present
Dynamics and Relaxation Times in Soft Nanomaterials. Our main goal is to explore the dynamics in soft nanocomposites (i.e. nanomaterials involving soft nanoparticles dispersed in a polymeric matrix) and to determine reliable relaxation times in these systems by means of broadband dielectric spectroscopy and small angle neutron scattering techniques. Theoretical models are combined with computer simulations to understand the observed experimental behaviour with special emphasis in new nanoscale effects.

PhD Fellowships

Remi Vincent
Université Paul Sabatier, Toulouse, France
01/11/2003–30/11/2009
Ions induced electron excitations in ferromagnetic materials. Interaction of ions with metals energy loss and stopping power. Study of metallic clusters. Response function.

Sara Capponi
University of Perugia, Italy
23/10/2005–Present
Dynamics of DNA and proteins by neutron scattering.

Iñigo Aldazabal Mensa
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/07/2006–12/08/2008
Electron emission in ion-surface grazing collisions; contributions to the convoy electrons. Wave packet propagation tecniques applied to STM systems.Laser induced electron emission in metallic surfaces.

Martin Brodeck
IFF-FZ, Forschungszentrum Jülich, Germany
01/10/2006–15/04/2008
Molecular dynamics simulations and neutron scattering measurements of the strongly decoupled dynamics which are exhibited by the different components of polyethyleneoxide (PEO)/polymethylmetacrylate (PMMA) blends which can differ up to 12 orders of magnitude in local relaxation times.

Olalla Pérez González
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
02/10/2006–Present
Plasmon excitations in metallic nanoparticles. Optical properties of nanostructured materials.

Xabier Zubizarreta Iriarte
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
16/10/2006–30/09/2008
Electronic structure calculations of metal surfaces with strong spin-orbit coupling.

Yon Sánchez Paisal
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
16/10/2006–09/03/2008
Electronic structure calculations in nanostructured systems with technological applications.

Juan Pablo Echeverry Enciso
Universidad del Valle, Cali, Colombia
28/08/2007–30/06/2008
Study of colective electronic excitations and dinamic of reduced symmetry systems.

Clément Riedel
Université Montpellier 2, France
05/09/2007–Present
Multiscale study of the dielectrics properties of matter from the nanoscopic scale to the macroscopic scale.

Nicolas Large
Université Paul Sabatier, France
01/10/2007–Present
Simulations of the optical properties of metallic nano-objects: acoustic phonons - surface plasmons coupling. Raman spectroscopy in low dimensional semiconductor structures.

Sandra Plaza García
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/10/2007–Present
Dynamics of funtionalized 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.

Marco Bernabei
Universita di Roma Tre, Italy
29/10/2007–Present
Molecular dynamics simulations of simple models for glass-forming polymers.

Marina Quijada Van den Berghe
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/11/2007–30/10/2009
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, Spain
01/12/2007–30/06/2008
Non-adiabatic processes in the adsorption of diatomic molecules on metal surfaces.

Carlos Etxeberria Arrondo
Universidad Pública de Navarra, Spain
01/01/2008–Present
Quantum dots based on magnetic semiconductors.

Giuseppe Foti
Universita Mediterranea di Reggio di Calabria, Italia
01/11/2008–30/06/2009
Electronic transport through molecular

Zakaria Mohammed Slimani
Centre Européen de Calcul Atomique et Moléculaire (CECAM), Lyon
24/02/2009–Present
Dynamics of diblock copolymers by computer simulations (Ph.D.) Computer simulations of self-assembly and slow dynamics in diblock copolymers

Roberto Pérez Aparicio
Universidad de Valladolid, Spain
01/09/2009–Present
Study of molecular dynamics in glass forming polymers by means of neutron scattering techniques and molecular dynamics simulations. In particular, this work focuses on the poly (ethylene propylene) (PEP) in order to study its molecular dynamics at local scales (atomic motions), large scales (chain dynamics), and also the crossover between them.

Asier Ozaeta Rodriguez
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain
01/12/2009–Present
Transport properties of superconducting weak links in the presence of a rf-field.

Visiting Researchers

Long visits

Prof. Eugene Krasovskii
Universität Kiel, Germany
07/01–30/03/2008
First-principles calculations of collective excitations in bulk metals.

Prof. Joseph R. Manson
Clemson University, USA
06/05–15/08/2008
Theoretical investigations of the microscopic structure and dynamical properties of surfaces.

Prof. Juan José Sáenz Gutierrez
Universidad Autónoma, Spain
01/06–31/07/2008, 01/06–30/07/2009
Nanophotonics. Modeling scanning probe microscopies.

Prof. Wolfgang Schattke
Universität Kiel, Germany
01/10–30/11/2008
Variational Quantum Montecarlo calculations of the electronic properties of solids and surfaces. Theory of photoemission in semiconductors and metals.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Italy
02/06–30/06/2008, 02/10–30/10/2008, 01/06–30/06/2009
Surface phonons and phase transitions.

Prof. Viktor Tugushev
RRC Kurchatov Institute, Moscow, Russia
03/04–27/06/2008
Magnetism in superlattices and spintronics.

Prof. Vladimir Menshov
RRC Kurchatov Institute, Moscow, Russia
15/05–15/08/2008
Confling mechanisms in digital alloys.

Prof. Sergey Eremeev
Institute of Strength Physics and Materials Sciences, Tomsk, Russia
01/06–30/08/2008, 03/07–30/09/2009
Phonons and electron-phonon coupling in quantum-well states of adlayers on metals.

Prof. Philippe Tordjeman
Université Montpellier 2, France
04/02–18/06/2008
Nanodielectric of polymer.

Prof. Amand Lucas
FUNDP, Namur, Belgium
30/09–30/10/2008, 03/09–30/11/2009
Condensed matter physics, surface sciences, electronic and atomic structures of reduced dimensionality systems structural biology.

Dr. Ilya Nechaev
Kostroma State University, Russia
22/06–19/09/2008, 21/06–16/09/2009
Electron excitations in ferromagnetic materials.

Prof. Norman March
University of Antwerpen, Belgium
08/04–08/06/2008, 15/04–14/06/2009
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.