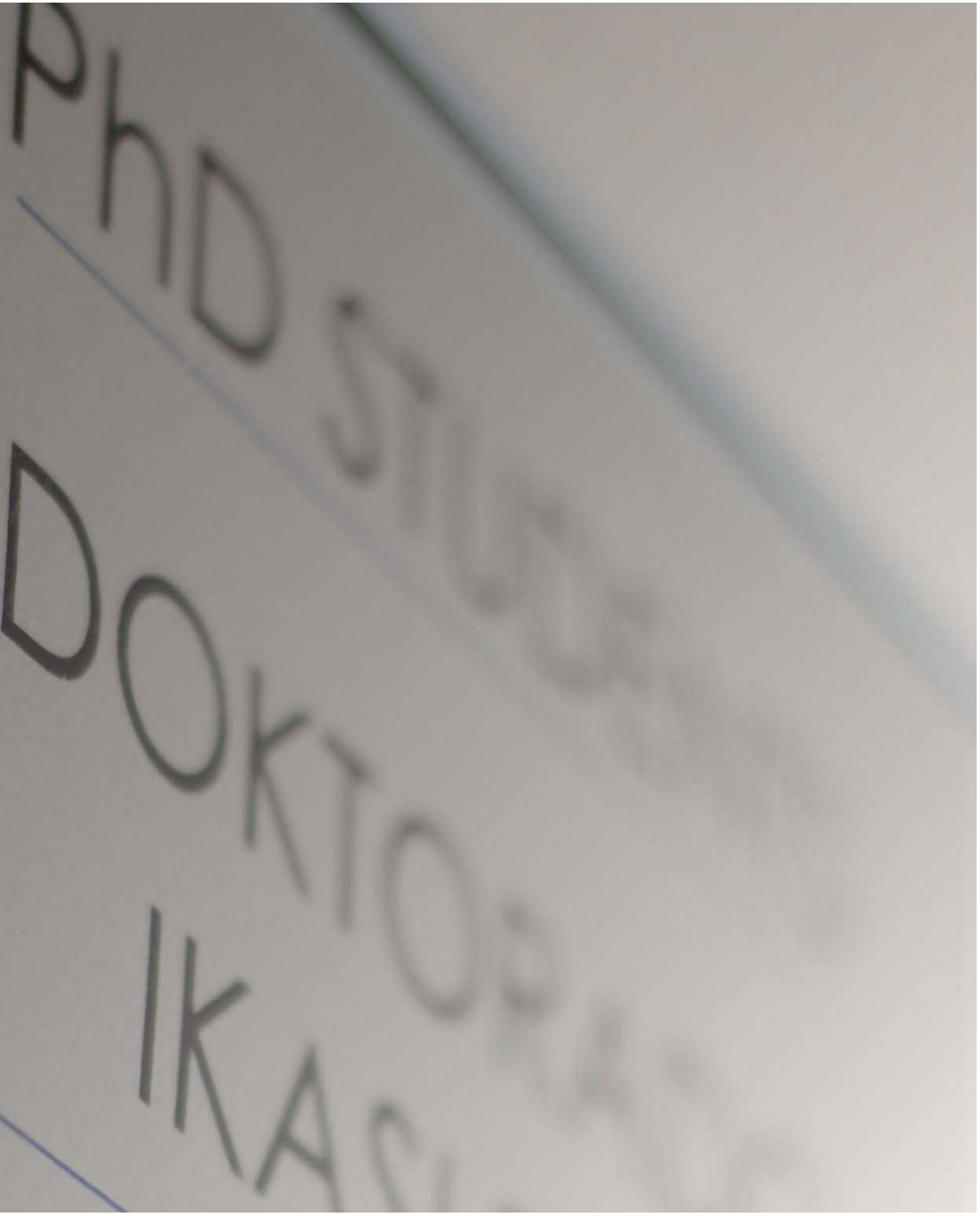

Researchers

Fellows Gipuzkoa

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. 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, nonequilibrium 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.

Dr. Maria Blanco Rey
University of Cambridge, United Kingdom
01/12/2010–Present
Metal oxide surface chemistry with applications in catalysis and physical properties of intrinsically chiral surfaces.

Postdoctoral Positions

Dr. Reidar Lund
IFF-FZ, Forschungszentrum Jülich, Germany
20/02/2006–15/10/2011
Dynamics in funcionalized polymers.

Dr. Dimas Garcia de Oteyza Feldermann
Max Planck Institute for Intelligent Systems, Stuttgart, Germany
01/09/2007–30/09/2010
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
02/09/2007–31/05/2010
Plastic deformation of gamma phase isotactic polypropilene in the plane-strain compression.

Dr. Dusan Racko
Polymer Institute, SAS, Slovak Republic
03/09/2007–31/08/2010
Molecular dynamics simulations in polymers.

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. Virginie Boucher
École Nationale Supérieure de Chimie de Lille, France
30/10/2008–31/10/2011
Dynamical properties at molecular scale in polymeric materials multi-component and/or nano-structured combining different experimental techniques, in particular, dielectric and mechanical spectroscopy. The possibility of using x-rays and neutron scattering is also envisaged.

Dr. Remi Busselez
Universite de Rennes, France
03/11/2008–30/09/2010
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. Ludovic Martin-Gronde
Université Bordeaux 1, France
01/09/2009–31/10/2011
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
Jawaharlal Nehru University, New Delhi, India
07/09/2009–31/07/2011
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
Universität Basel, Switzerland
01/11/2009–31-08-2011
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.

Dr. Maia García Vergniory
Lawrence Berkeley National Laboratory, USA
01/01/2010–31-12-2011
First-principles calculations of contact effect on quantum transport.

Dr. Mario Piris Silvera
UPV/EHU, Spain
01/01/2010–31/12/2010
Further development of PNOF natural orbital functional.

Dr. Duncan J. Mowbray
Center for Atomicscale Materials Design, Technical University of Denmark, Denmark
09/04/2010–31-3-2011
Time-resolved oxyde mediated photocatalisis.

Dr. Pawel Rejmak
Institute of Catalysis and Surface Chemistry of Polish Academy of Science, Poland
02/06/2010–Present
First-principles calculations on nanostructures.

Dr. Remi Avriller
Universidad Autónoma de Madrid, Spain
06/10/2010–30/09/2011
Inelastic quantum transport properties of nanoscale objects.

Dr. Paulina Gonzalez-Morelos
Cornell University, New York, USA
25/10/2010–31/12/2010
TDDFT study of the energy loss of swift ions in solids.

Dr. Ester Sola Badia
University College London, United Kingdom
03/11/2010–27/03/2011
Ab initio study of the structural, electronic and optical properties of nanoparticle-filled molecular cages.

Dr. Vasse Chis
University of Göteborg, Sweden
15/11/2010–Present
First-principle calculations of vibrations and electron-phonon interaction in heavy materials.

Dr. Iñigo Garcia Yoldi
Instituto de Ciencia y Tecnología de Polimeros, CSIC Madrid, Spain
01/03/2011–Present
Simulation of confined polymers.

Dr. Patrizia Borghetti
Universita Cattolica del Sacro Cuore, Brescia, Italy
07/04/2011–07/04/2012
Physical chemistry of interfaces in organic solar cells.

Dr. Alvise Verso
Ulm University, Germany
01/05/2011–Present
Readout of a superconducting qubit: a problem of quantum escape processes for driven systems.

Dr. Alejandro Miccio
Facultad de Ingeniería - INTEMA, Mar del Plata, Argentina
21/07/2011–Present
Local Dielectric Spectroscopy by means of AFM.

Dr. Eithiraj Rajagopal Dashinamoorthy
Anna University, India
18/08/2011–Present
Computational solid state spectroscopy.

Temporary Contract Position

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 San Petersburg, Russia
17/07/2009–31/07/2010
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, Donostia-San Sebastián, Spain
16/11/2009–31/08/2010
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 Students

Sara Capponi
University of Perugia, Italy
23/10/2005–30/06/2011
Dynamics of DNA and proteins by neutron scattering.

Olalla Pérez González
Facultad de Ciencia y Tecnología, UPV/EHU, Spain
02/10/2006–Present
Plasmon excitations in metallic nanoparticles. Optical properties of nanostructured materials.

Clément Riedel
Université Montpellier 2, France
05/09/2007–09/09/2011
Multiscale study of the dielectrics properties of matter from the nanoscopic scale to the macroscopic scale.

Nicolas Large
Université Paul Sabatier, Toulouse, France
01/10/2007–31/10/2011
Interaction of localized plasmons and acoustic vibrations in metallic nanostructures.

Sandra Plaza García
UPV/EHU, Spain
01/10/2007–31/12/2011
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, Roma, Italy
29/10/2007–Present
Molecular dynamics simulations of simple models for glass-forming polymers.

Carlos Etxeberria Arrondo
Universidad Pública de Navarra, Spain
01/01/2008–31/03/2010
Quantum dots based on magnetic semiconductors.

Zakaria Mohammed Slimani
Centre Européen de Calcul Atomique et Moléculaire (CECAM), Lyon, France
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
01/09/2009–31/07/2010
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
UPV/EHU, Spain
01/12/2009–30/09/2010
Transport properties of superconducting weak links in the presence of a rf-field.

Irma Pérez Baena
UPV/EHU, Spain
08/03–31/08/2010
Dynamics and phase diagrams for soft nanoparticles and all-polymer nanocomposites thereof.

Mohamed Ameen Poyli
Bharathidasan University, Tiruchirappalli Tamil Nadu, India
01/06/2010–Present
Photonic Nanoantennas.

Elixabete Goiri Little
UPV/EHU, Spain
01/07/2010–Present
Tunneling microscopy and spectroscopy of molecules on metals at 1 K.

Natalia Koval
Adyghe State University, Russia
15/07–30/09/2010
Interacción entre pequeñas moléculas y superficies metálicas: reactividad y contribuciones no adiabáticas.

Alison Crawford Uranga
UPV/EHU, Spain
01/08/2010–31/12/2011
Non.adiabatic effects in the electronic and ionic response of molecules within the time-dependent density functional theory: development of new exchange and correlation functionals.

Mario Lechner
Johannes Kepler Universität Linz, Austria
01/09/2010–Present
Design and self-assembly of polymer-based nanoparticles by computer simulations.

Elton José Gomes dos Santos
CFM-CSIC, San Sebastián, Spain
01/01–21/10/2011
First-principles study of the electronic and magnetic properties of functionalized carbon nanostructures.

Alexander Correa Aristizabal
Universidad del Valle, Cali, Colombia
21/6/2011–Present
Studies at the nanoscale of interfaces for biosensor and solar cell applications.

Rubén González Moreno
Instituto de Ciencia de Materiales de Madrid, CSIC, Spain
27/07/2011–Present
Properties and organization of protoporpyrin IX molecules on metal and oxide surfaces.

Mikolaj Kajetan Schmidt
Copernico University, Torun, Poland
13/10/2011–Present
Radiative decay of emitters in the presence of magnetic dipoles.