

# Researchers

## Fellows Gipuzkoa

**Dr. Rubén Esteban Llorente**

11/03/2013–31/12/2016

Quantum plasmonics.

**Dr. Maia Garcia Vergniory**

01/06/2013–04/09/2016

Electronic and magnetic properties in ordered and disordered topological insulators.

**Dr. Peter Koval**

25/11/2013–Present

Development of MBPT with localized orbitals.

**Dr. Aitzol Garcia Etxarri**

01/11/2014–Present

Nanophotonics theory.

## Senior Positions

### Dr. Irina Sklyadneva

Electron-phonon coupling in the 3D topological isolators and Weil semiconductors as well as and in ultrathin lead and indium films on the Si substrate (superconductivity).

### Prof. Vladimiro Mújica Hernandez

Charge and spin transfer at nano-interfaces. Reformulation of Marcus theory using the molecular polarizability as fundamental variable.

## Postdoctoral Positions

### Dr. Stepan Tsirkin

State University of Tomsk, Russia  
06/12/2012–04/09/2016  
Magnetic proximity effect in the layered structures.

### Dr. María de Gracia Retamosa Hernández

Facultad de Química, UPV/EHU, Donostia / San Sebastián, Spain  
01/07/2013–31/01/2016  
Remote structural effects in unnatural amino acids.

### Dr. Mikhail Otrokov

State University of Tomsk, Russia  
17/07/2013–31/12/2016  
Topological insulators.

### Dr. Iosune Arrastia Basalo

Facultad de Química, UPV/EHU, Donostia / San Sebastián, Spain  
01/08/2013–Present  
Multiple spin state reactivity in Fe-containing complexes and enzymes.

### Dr. Elena Formoso Estensoro

Università della Svizzera Italiana, Lugano, Switzerland  
01/02/2014–31/12/2016  
Unveiling biochemical relevant structural conformations of the aluminum cation amyloid-beta peptide complex.

### Dr. Federica Lo Verso

Material Physics Center, MPC, Donostia / San Sebastián, Spain  
01/02/2014–Present  
Structure and dynamics of complex materials based on polymers.

### Dr. Rémi Pétuya

Institut des Sciences Moléculaires, Université Bordeaux, France  
01/10/2014–30/09/2016  
Characterization of structural and electronic properties of molecular overlayers on metal surfaces.

### Dr. Romain Dupuis

CEMES/CNRS, Toulouse, France  
10/12/2014–Present  
Computational studies on calcium silicate hydrates.

### Dr. Guillaume Vasseur

Institut Jean Lamour, Université de Lorraine-CNRS, France  
05/01/2015–08/08/2016  
Physics and chemistry of curved crystal surfaces.

### Dr. Joseba Alberdi Rodriguez

Facultad de Informática, UPV/EHU, Donostia / San Sebastián, Spain  
01/07/2015–Present  
Morfokinetics: development of computational techniques for the analysis of CVD growth of new 2D materials.

### Dr. Marta Pelc

Nicolaus Copernicus University, Torun, Poland  
01/12/2015–Present  
Topological defects on carbon like nanostructures.

### Dr. Omjyoti Dutta

University of Arizona, Tucson, Arizona, USA  
01/01/2016–Present  
Quantum matter and quantum simulations at the interface of optics and solid state physics.

### Dr. Daniel Martinez Tong

Université Libre de Bruxelles, Belgium  
11/01/2016–Present  
Local dielectric spectroscopy by AFM. Application to polymer based materials.

### Dr. Pablo Aguado Puente

CIC nanoGUNE  
15/02–30/06/2016  
Coupling of ferroic nanoscale films with interfacial two dimensional electron gases in oxides.

### Dr. Mathias Ljungberg

Phillips Universität Marburg, Germany  
01/04/2016–Present  
Model calculations of solid organic/inorganic interface.

**Dr. Carlos Garcia Fernandez**

Instituto Superior de Ciencias y Tecnologías Nucleares, La Habana, Cuba  
20/04/2016–Present

Development of transport methods based on Wannier function.

**Dr. Mario Zapata Herrera**

Universidad de los Andes, Bogotá, Colombia  
01/07/2016–Present

Quantum and classical approaches to the optical response of metallic nanostructures.

**Dr. Pawel Nita**

Marie Curie-Sklodowska University, Lublin, Poland  
01/08/2016–Present

Functional materials synthesized by surface-supported chemistry under vacuum.

**Dr. Jon Iñaki Mujika**

Facultad de Química, UPV/EHU, Donostia / San Sebastián  
16/08/2016–Present

Molecular dynamics of membrane structure.

**Dr. Aleksander Terentjev**

Instituto Nanoscienze-CNR, Euromediterranean Center for Nanomaterial Modelling and Technology (ECMT), Lecce, Italy  
01/09/2016–Present

Time dependent density functional theory beyond the local density approximation.

**Dr. Jorge Budagosky Marcilla**

Universidad de Zaragoza, Spain  
01/10/2016–Present

Computational solid state spectroscopy.

**Dr. Victor Escobedo Bermudez**

Universidad de Salamanca, Spain  
01/10/2016–Present

Literature and science.

**Dr. Nuno De Sousa**

Universidad Autónoma de Madrid, Spain  
08/11/2016–Present

Light scattering, emission rates and optical forces in colloidal suspensions.

**Dr. Maxim Ilin**

Materials Physics Center CSIC-UPV/EHU, Donostia / San Sebastián, Spain  
16/12/2016–Present

Upgrade of MOKE setup to add up the capability for as-susceptibility measurements.

## PhD Students

**Anton Xose Brion Rios**

18/02/2016–Present

Theoretical study on the molecular adsorption and self-organization on substrates of different nature.

**Dino Novko**

25/09/2013–Present

Non-adiabatic effects in the interaction of metal surfaces with atoms and small molecules.

**Oihana Galparsoro Larraza**

01/10/2013–30/09/2016

Phonon and electron excitations in diatom abstraction from metallic surfaces.

**Bernhard Kretz**

09/06/2014–Present

Electronic and transport properties of graphenic nanostructures.

**Lucía Ortega Álvarez**

12/01/2015–Present

Structure and dynamics of silica filled rubber compounds.

**Natalia Koval**

21/01/2015–19/01/2016

Time-dependent density functional theory calculations of the energy loss of particles in metallic media.

**Néstor Merino Díez**

01/09/2015–Present

Tema de investigación: Functional materials synthesized by surface-supported chemistry under vacuum.

**Mattin Urbieto**

01/01–10/04/2016

Plasmonics of metallic nanoparticles and hybrid nanostructures.

**Mohamed Ahmed Nosir**

01/01–30/12/2016

Theoretical study of the dynamics of nitrogen atoms and molecules interacting with iron surfaces.

**Jon Lafuente Bartolomé**

01/01/2016–Present

Relativistic corrections and spinorial structure of the response function in 2D systems.

**Bogusz Bujnowski**

01/04/2016–Present

Quantum transport in hybrid structure with semimetals, excitonic insulators and superconductor.

**Federico Marchesin**

14/07/2016–31/12/2016

Ab initio plasmonics using LCAO basis sets.

**Jordan Ochs**

01/10/2016–Present

Synthesis of cyclic polymers.

**Jorge Olmos Trigo**

01/10/2016–Present

Theory and modelling of topological photonic materials.

**Evgenia Rusak**

01/10–16/12/2016

Quantum description of plasmonic systems and their coupling with single emitters.

**Cristina Sanz Fernandez**

01/10–14/12/2016

Light emission and propagation in all-dielectric photonic structures.

**Olatz Uranga Barandiaran**

15/11/2016–Present

Theoretical and computational studies of excited states in molecules and aggregates.

Functional materials synthesized by surface-supported chemistry under vacuum.

## Internships

**Daniel Camacho Piris**

Facultad de Informatica, UPV/EHU, Donostia / San Sebastián, Spain

01/06–31/08/2016

Batch system management

**Gonzalo Oyarzabal Insausti**

Facultad Informática, UPV/EHU, Donostia / San Sebastián, Spain

01/06–31/08/2016

Cluster monitorization.

**Olatz Romeo Amiama**

Facultad de Informática, UPV/EHU, Donostia / San Sebastián, Spain

01/06–31/08/2016

Unattended instalation.

**Alvaro Martinez Dominguez**

Facultad de Ciencia y Tecnología, Leioa, UPV/EHU, Spain

06/06–05/08/2016

Light scattering and optical forces on nanoparticles.

**Asier Insausti Gonzalez**

Facultad de Ciencia y Tecnología, UPV/EHU, Leioa, Spain

13/06–12/08/2016

Massless Kane fermions in the topological insulator HgCdTe.

**Javier López Piqueres**

Universidad Autónoma de Madrid, Spain

20/06–19/08/2016

Trapping matter with nano-structures.

**Unai Muniain Caballero**

Facultad de Ciencia y Tecnología, UPV/EHU, Donostia / San Sebastián, Spain

20/06–19/08/2016

Atomic scale engineering of graphene nanostructures.

**Alvaro Cuartero Gonzalez**

Universidad Autónoma de Madrid, Spain

24/06–23/08/2016

Optical antennas to control light at the nanoscale.

**Lucía Gonzalez Rosado**

Universidad Autónoma de Madrid, Spain

27/06–27/08/2016

Topological invariants of Majorana fermions in a chain of magnetic atoms.

**Rodrigo Asensio Perea**

Facultad de Ciencia y Tecnología, UPV/EHU, Leioa, Spain

01/07–31/08/2016

Optical antennas to control the angular momentum of light.

**Juan Reino González**

Universidad Autónoma de Madrid, Spain

04/07–04/09/2016

Development of density functionals in DFT.

**Nerea Jiménez Irurzun**

Facultad de Química, UPV/EHU, Donostia / San Sebastián, Spain

01/08–30/09/2016

Topological gels based on cyclic polymers.

**Sofía Sanz**

Universidad Autónoma de Madrid, Spain

05/09–31/10/2016

Quantum transport in nanoscale devices.

**Igor Cortés Cejudo**

Facultad de Informática, UPV/EHU, Donostia / San Sebastián, Spain

03/10–31/01/2017

Virtual machines cluster installation.

**Miriam Rico Medina**

Facultad de Informática, UPV/EHU, Donostia / San Sebastián, Spain

03/10–31/01/2017

Energy saving system for the computer clusters.

**Ikerbasque Research Professors****Prof. Andreas Heidenreich**

Computer simulations of nanoplasma formation, Coulomb explosions and nuclear fusion induced by ultraintense and ultrashort laser pulses.

Computer simulations of pump-probe signals.

**Prof. Andrey Kazanskiy**

Investigation of subfemto-atto second processes in gases and solids caused by ultrashort laser pulses. Investigation of dynamics of electrons in surface and image states of noble metal and their interaction with adsorbates.

**Prof. Eugene Krasovskii**

Electronic structure of nanosystems, surfaces and interfaces. Attosecond time resolved photoelectron spectroscopy to study the dynamics of electronic excitations. Full dielectric function of bulk crystals, surfaces and two dimensional nanostructures. Development of new computational methods of the density functional theory.

**Prof. Mario Piris Silveira**

Energy functional method development. Computational modelling of semiconductor nanocluster and molecular solid phases and polymorphism.

**Prof. Slawomir Grabowski**

Analyses of intra- and intermolecular interactions in the gas phase, ab initio and DFT calculations as well as the use of the other theoretical methods as for example Quantum theory of atoms in molecules and natural bond orbitals approach. Studies on crystal structures of organic and organometallic compounds, analyses of different Lewis acid-Lewis base interactions (mostly hydrogen bonding) influencing geometries of species

constituting crystals and influencing arrangement of molecules and/or ions in crystals, the use of theoretical methods for these analyses as well as statistical methods as for example factor analysis.

**Prof. Vyacheslav Silkin**

Ultrafast dynamics of the one-particle and collective electronic excitations in metals and their surfaces. The study of electronic excitations at adsorbates on metal surfaces.

**Prof. Thomas Frederiksen**

Nanoelectronics - theory and simulation.

**Prof. Geza Giedke**

Quantum Information and Quantum Optics: Implementations of QIP in atomic and solid-state systems.

**Prof. Dimas Garcia de Oteyza Fieldman**

Physical chemistry phenomena in organic materials and organic-inorganic interfaces.

**Prof. Juan José Saenz Guitierrez**

Light scattering in colloidal suspensions.

**Prof. Fabienne Barroso Bujans**

Novel complex-shaped cyclic polymers, from synthesis to physical properties. Devices and nanodevices based on cyclic polymers/graphene hybrid materials.

## Ikerbasque Research Fellows

**Dr. Arantzazu Garcia Lekue**

01/11/2012–Present

Modeling electron transport at the nanoscale.  
Theoretical investigation of electron processes  
at nanostructured surface.

**Dr. María José Cabrera San Félix**

01/11/2012–Present

Molecular level understanding of the interaction  
of molecules (particularly water) with surfaces and  
their self-assembly to form extended structures.  
Electronic and structural properties of clean and  
decorated surfaces: surface reconstructions and  
chemical reactivity.

**Dr. Dario Bercioux**

01/10/2014–Present

Quantum transport in nanostructures.

## DIPC Associates

Prof. Javier Aizpurua CSIC

Dr. Maite Alducin CSIC

Dr. Ignacio Arganda-Carreras UPV/EHU

Prof. Andrés Arnau UPV/EHU

Prof. Emilio Artacho CIC nanoGUNE

Dr. Andrés Ayuela, CSIC

Prof. Rolindes Balda UPV/EHU

Dr. Aitor Bergara UPV/EHU

Dr. Sebastian Bergeret CSIC

Dr. Maria Blanco UPV/EHU

Dr. Igor Campillo Euskampus

Dr. David Casanova UPV/EHU

Dr. Miguel Ángel Cazalilla CSIC

Prof. Eugene Chulkov UPV/EHU

Prof. Juan Colmenero UPV/EHU

Prof. Fernando Cossio UPV/EHU

Dr. Fernando Delgado UPV/EHU

Dr. Ricardo Díez Muiño CSIC

Prof. Pedro Miguel Echenique UPV/EHU

Dr. Asier Eiguren UPV/EHU

Dr. Ion Errea UPV/EHU

Prof. Joaquín Fernández UPV/EHU

Dr. Idoia García de Gurtubay UPV/EHU

Dr. Maia Garcia Vergniory UPV/EHU

Prof. Francisco José García Vidal UAM

Dr. Miguel Angel Gosalvez UPV/EHU

Dr. Iñaki Juaristi UPV/EHU

Dr. Aritz Leonardo UPV/EHU

Dr. Xabier Lopez UPV/EHU

Dr. Nicolás Lorente CSIC

Dr. Eduard Matito UPV/EHU

Dr. Jon M. Matxain UPV/EHU

Dr. Jose M. Mercero UPV/EHU

Dr. Angel Moreno CSIC

Prof. Enrique Ortega UPV/EHU

Prof. Juan Ignacio Pérez UPV/EHU

Prof. José Maria Pitarke UPV/EHU

Prof. Yuri Rakovich UPV/EHU

Dr. Elixabete Rezabal UPV/EHU

Prof. Alberto Rivacoba UPV/EHU

Dr. Celia Rogero CSIC

Prof. Ángel Rubio UPV/EHU

Dr. Daniel Sánchez Portal CSIC

Dr. Ane Sarasola UPV/EHU

Dr. Frederik Schiller CSIC

Dr. Gustavo Ariel Schwartz CSIC

Prof. Ivo Souza UPV/EHU

Prof. Jesus M. Ugalde UPV/EHU

Prof. Lucia Vitali UPV/EHU

Dr. Nerea Zabala UPV/EHU