

# Researchers

## Fellows Gipuzkoa

**Dr. Peter Koval**

25/11/2013–Present

Development of MBPT with localized orbitals.

**Dr. Aitzol Garcia Etxarri**

01/11/2014–Present

Nanophotonics theory.

## Senior Position

**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).

## Postdoctoral Positions

**Dr. Miren Iosune Arrastia Basalo**

01/08/2013–Present

Multiple spin state reactivity in Fe-containing complexes and enzymes.

**Dr. Federica Lo Verso**

01/02/2014–31/01/2017

Structure and dynamics of complex materials based on polymers.

**Dr. Romain Dupuis**

10/12/2014–09/12/2017

Computational studies on calcium silicate hydrates.

**Dr. Joseba Alberdi Rodriguez**

01/07/2015–Present

Morfokinetics: development of computational techniques for the analysis of CVD growth of new 2D materials.

**Dr. Marta Pelc**

01/12/2015–Present

Topological defects on carbon like nanostructures.

**Dr. Omjyoti Dutta**

01/01/2016–31/12/2017

Quantum matter and quantum simulations at the interface of optics and solid state physics.

**Dr. Daniel Martinez Tong**

11/01/2016–Present

Local dielectric spectroscopy by AFM. Application to polymer based materials.

**Dr. Mathias Ljungberg**

01/04/2016–31/03/2017

Model calculations of solid organic/inorganic interface.

**Dr. Carlos Garcia Fernandez**

20/04/2016–Present

Development of transport methods based on Wannier function.

**Dr. Mario Zapata Herrera**

01/07/2016–Present

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

**Dr. Pawel Nita**

01/08/2016–31/07/2017

Functional materials synthesized by surface-supported chemistry under vacuum.

**Dr. Jon Iñaki Mujika**

16/08/2016–Present

Molecular dynamics of membrane structure.

**Dr. Aleksander Victorovich Terentjev**

01/09/2016–Present

Time dependent density functional theory beyond the local density approximation.

**Dr. Jorge Budagosky Marcilla**

01/10/2016–Present

Computational solid state spectroscopy.

**Dr. Victor Escobedo Bermudez**

01/10/2016–27/10/2017

Literature and science.

**Dr. Nuno De Sousa**

08/11/2016–07/06/2017

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

**Dr. Maxim Ilin**

16/12/2016–Present

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

**Dr. Luca Bergamini**

01/01–31/12/2017

Optical response of nano-antennas and novel materials.

**Dr. Beatriz Robles**

01/01/2017–Present

Dynamic properties of concentrated solutions of single chain nanoparticles.

**Dr. Yao Zhang**

01/01–31/12/2017

Atomistic description of surface enhanced raman spectroscopy.

**Dr. Rafael Grande Aztatzi**

13/03/2017–Present

Molecular dynamics of Al protein interactions.

**Dr. Deung Jang Choi**

01/05/2017–Present

Magnetic states on superconducting surfaces.

**Dr. Luciano Colazzo**

26/06/2017–Present

Functional materials synthesized by surface-supported chemistry under vacuum.

**Dr. Susana Velasco**

10/07–07/09/2017

Developing catalytic and photocatalytic assays under biologically relevant conditions.

**Dr. Jens Herwig Brede**

01/09–31/12/2017

Physical chemical reactions at surfaces: physico-chemical aspects.

**Dr. Pedro Brandimarte Mendonca**

01/10/2017–Present

Electronic structure and quantum transport in graphene based nanostructures and networks.

**Dr. Alejandro Rivero Santamaría**

09/10/2017–Present

Dynamics of elementary reactive processes at surfaces.

**Dr. Jhon Wilfer Gonzalez Salazar**

01/11/2017–31/01/2018

Electronic and magnetic properties of 2D materials and small clusters.

**Dr. Xavier Monnier**

15/11/2017–Present

Ultra dense/low energy state glasses by aging nanostructured polymers.

**Dr. Paula Malo de Molina Hernandez**

15/12/2017–Present

All polymer nano composites: effect of soft nano objects on polymer structure and dynamics.

## PhD Students

**Anton Xose Brion Rios**

06/02/2013–Present

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

**Dino Novko**

25/09/2013–10/04/2017

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

**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.

**Néstor Merino Díez**

01/09/2015–Present

Functional materials synthesized by surface-supported chemistry under vacuum.

**Jon Lafuente Bartolomé**

01/01/2016–12/03/2017

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.

**Jordan Ochs**

01/10/2016–Present

Synthesis of cyclic polymers.

**Jorge Olmos Trigo**

01/10/2016–Present

Theory and modelling of topological photonic materials.

**Olatz Uranga Barandiaran**

15/11/2016–22/01/2017

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

**Irene Casademont**

01/01/2017–22/01/2017

Computational studies of molecular photosensitizers.

**María Eugenia Sandoval Salinas**

11/01/2017–28/02/2017

Photophysical processes in complex systems.

**Peio Garcia Goiricelaya**

01/02/2017–Present

Spinorial structure of the electron-phonon interaction in surfaces with strong relativistic corrections.

**Donaldi Mancelli**

03/02/2017–Present

Experimental and theoretical analysis of simple compounds under shock-wave compression

**José Reina Galvez**

01/03/2017–15/04/2017

DFT calculations of the electronic structure of Co and Fe atoms on MgO.

Calculations of multiplets, with SOC. Derivation of an "effective spin Hamiltonian".

**María Blanco De Paz**

27/03/2017–Present

Spin orbit interactions in photonic systems.

**Juan Gurruchaga Pereda**

03/04/2017–Present

Photocatalytic upconverting nanomaterials for metal based photochemotherapy.

**Moritz Müller**

09/06/2017–Present

Lifetimes of HOMO and LUMO states of organic molecules relevant for organic photovoltaics on different substrates.

**Xianpeng Zhang**

11/07/2017–Present

Spin and charge transport in low dimensional systems and hybrid structures.

**Alvaro Nodar Villa**

01/09/2017–Present

Quantum approaches to the interaction of molecules and plasmonic excitations in nanophotonics.

**Mikel Olano Aramburu**

01/09/2017–Present

Quantum information processing with electrons and phonons in semiconductors.

**Xabier Telleria Allika**

04/09/2017–Present

Statically screened potentials, Hookean systems and quantum dots.

**Sofia Sanz Wuhl**

07/09/2017–Present

Theory of quantum transport in graphene based nanostructure networks.

**Antton Babaze**

01/10/2017–Present

Quantum approaches to the interaction of molecules and plasmonic excitations in nanophotonics.

**Raúl Guerrero Avilés**

27/10/2017–Present

Adsorbing atoms and molecules on van der Waals heterostructures.

**Mohammed Sabri Gamal Mohammed**

01/11/2017–Present

Functional materials synthesized by surface-supported chemistry under vacuum.

**Haritz Garai Marin**

15/11/2017–Present

Relaxation of electronic states of magnetic ad-atoms at surfaces considering numerical renormalization group (NRG).

**Iñigo Robredo Magro**

16/11/2017–Present

Looking for new fermions in conventional crystals.

**Mikel Arruabarrena**

01/12/2017–Present

TDDFT approach for the direct calculation of exciton binding energies.

## Internships

**Igor Cortés Cejudo**

UPV/EHU

03/10/2016–31/01/2017

Virtual machines cluster Installation.

**Miriam Rico Medina**

UPV/EHU

03/10/2016–31/01/2017

Energy saving system for the computer clusters.

**Aritz Olea Zubikarai**

UPV/EHU

01/02–31/03/2017

Security appliance installation for the I2basque network.

**Ivan Escalante Crespan**

UPV/EHU

01/02–31/05/2017

Monitoring HPC Clusters.

**Iker Moya González**

UPV/EHU

01/02–31/05/2017

Monitoring micro-computing equipment.

**Edorta Beitia Lobato**

UPV/EHU

15/05–28/07/2017

Installation and configuration of a mail server for sensors & queue systems.

**Silvia García García**

UPV/EHU

15/05–14/07/2017

Installation and configuration of advertising displays.

**Edgar Orosa Paz**

UPV/EHU

01/06–31/07/2017

Improvement of the utilization of DIPC computational resources.

**Josu Salinas Colina**

UPV/EHU

01/06–31/07/2017

Development of open-source software for the unsupervised segmentation of bio-medical images.

**Maialen Galdeano Fraile**

UPV/EHU

08/06–07/08/2017

DFT calculations of charged graphene flakes.

**Unai Muniain Caballero**

UPV/EHU

12/06–11/08/2017

Quantum effects in plasmonic gratings.

**Martín Callejo Arroyo**

UPV/EHU

15/06–14/08/2017

Quantum transport in graphene-based nanodevices.

**Jon Lasa Alonso**

Universidad de Salamanca

15/06–15/08/2017

Sensing capabilities of nanophotonic devices.

**Joseba Goikoetxea Perez**

Universidad Autónoma de Madrid

03/07–31/08/2017

Quantum interference effects due to spin fields in mesoscopic rings.

**Jaime Saez Mollejo**

Universidad Autónoma de Madrid

03/07–03/09/2017

Simulation of electronic properties in graphene nanostructures.

**Silvia Escayola Gordils**

Universidad de Gerona

15/07–15/09/2017

Short-range DFT correlation within the RAS-SF method.

**Martí Gimferrer Andrés**

Universidad de Gerona

15/07–15/09/2017

Electron correlation in intracules functions of the pair density.

**Adriana Faraone**

University of Bologna, Italy

26/07–26/09/2017

Development of photoactivatable nanomaterials for chemotherapy.

**Daniel Ruiz Fulgencio**

UPV/EHU

01/08–30/09/2017

Isolation of cyclic oligomers of poly(ethylene oxide) from blends by selective intercalation into graphite oxide.

## 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 subfemtosecond 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 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.

### Prof. Luca Salassa

Development of photoactivatable anticancer metal complexes and nanomaterials. Experimental and computational inorganic photochemistry.

### Prof. Denis Vyalikh

Photoemission measurements of magnetic surface states.

## Ikerbasque Research Fellows

Dr. Dario Bercioux

01/10/2014–Present

Quantum transport in nanostructures.

Dr. Rubén Esteban Llorente

01/01/2017–Present

Tema de investigación: Quantum plasmonics.

## Ikerbasque Research Associates

Dr. Marek Grzelczak

01/09/2017–Present

Synthesis and self-assembly of plasmonic nanoparticles for photochemical applications.

Dr. Arantzazu Garcia Lekue

01/11/2017–Present

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

Dr. Paola Ferrario

01/12/2017–Present

Neutrino physics.

## 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. Sara Barja UPV/EHU

Dr. Aitor Bergara UPV/EHU

Dr. Sebastian Bergeret CSIC

Dr. Maria Blanco UPV/EHU

Dr. Igor Campillo Euskampus

Dr. Daniele Cangialosi CSIC

Dr. David Casanova UPV/EHU

Dr. Miguel Ángel Cazalilla CSIC

Dr. Silvina Cerveny CSIC

Prof. Eugene Chulkov UPV/EHU

Dr. Martina Corso CSIC

Prof. Fernando Cossio UPV/EHU

Dr. David De Sancho UPV/EHU

Dr. Asier Eiguren UPV/EHU

Dr. Ion Errea UPV/EHU

Prof. Joaquín Fernández UPV/EHU

Dr. Idoia García de Gurtubay UPV/EHU

Prof. Francisco José García Vidal UAM

Dr. Miguel Angel Gosalvez UPV/EHU

Dr. Iñaki Juaristi UPV/EHU

Dr. Stefan Kurth 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

Dr. Miguel Moreno Ugeda UPV/EHU

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

Dr. Ilya Tokatly UPV/EHU

Prof. Jesus M. Ugalde UPV/EHU

Prof. Lucia Vitali UPV/EHU

Dr. Nerea Zabala UPV/EHU