ACTIVITY REPORT 2016

CFM

Centro de Física de Materiales

Materialen Fisika Zentroa

Materials Physics Center

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CSIC
Consejo Superior de Investigaciones Científicas

Universidad del País Vasco
Euskal Herriko Unibertsitatea

MPC
Materials Physics Center

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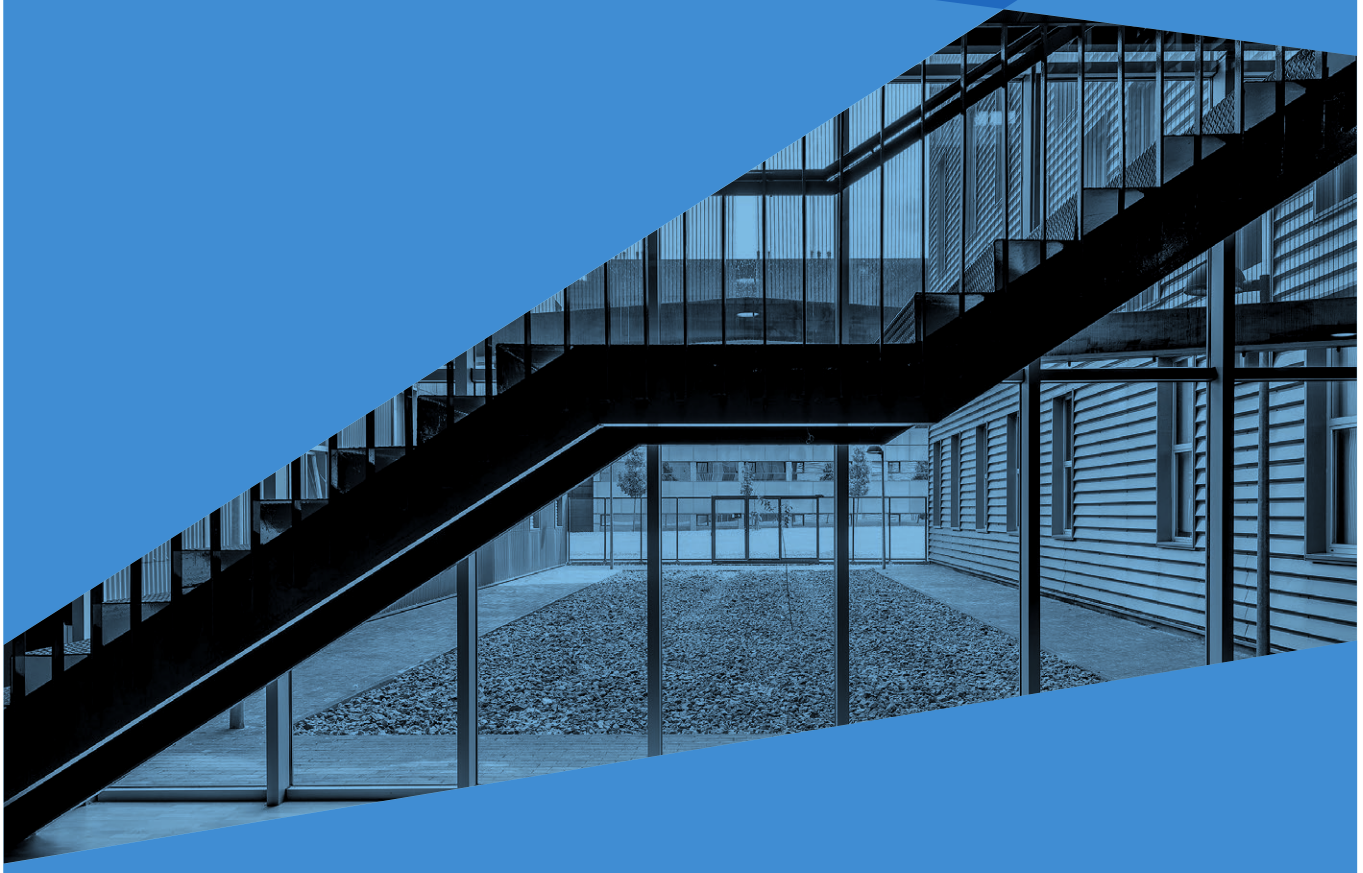


SUMMARY

SUMMARY

FOREWORD

"At CFM we take a close look into matter´s structure at the nanoscale to get a deeper understanding of electronic, magnetic, optic and dielectric properties of novel materials"

Centro de Física de Materiales-Materials Physics Center – CFM-MPC operates at the forefront of Materials Science, pushing the limits of this discipline to the frontiers of knowledge and providing high-quality training for new generations of scientists and technologists.

CFM is a joint Center of *Consejo Superior de Investigaciones Científicas (CSIC)* and *Universidad del País Vasco – Euskal Herriko Unibersitatea (UPV/EHU)*. Since year 1999, these two flagship institutions have merged forces in order to rationalize, optimize and multiply the effect of their investments in this area of research. Since 2009, the Basque Government has joined this long term commitment by distinguishing CFM as a Basque Excellence Research Centre (BERC) through the joint Association Materials Physics Center (MPC).

CFM is located at Ibaeta Campus in Donostia – San Sebastián, at the very core of a thrilling research community focused on a variety of aspects of Materials Sciences, with reference institutions in very close proximity in the campus, such as CIC nanoGUNE, POLYMAT, Donostia International Physics Centre (DIPC), or different University Departments of the Faculty of Chemistry at UPV/EHU, with whom CFM works in perfect synergy.

Within this stimulating environment, CFM plays a central role, representing its founding institutions

and hosting a stable critical mass of world-class research groups focused on fundamental materials science. CFM activity is developed by a core of scientists, boosting cooperation and development of multidisciplinary research in materials science that ranges from physical chemistry to surface physics, through photonics, condensed and soft matter physics, which has materialized in an important track of high profile scientific publications and has attracted a significant amount of competitive funding of scientific projects.

The structure of CFM in four main research lines, (i) Chemical physics of complex materials, (ii) electronic properties at the nanoscale, (iii) photonics and (iv) polymers and soft matter, has proven to be an efficient scientific framework, where experimentalist and theoreticians with different backgrounds exchange ideas and pursuit challenging scientific goals, and also where students receive up-to-date training and have the chance to interact with world-class researchers.

During 2016, CFM has continued its activity as a center of excellence in Materials Science producing more than 200 publications in peer-reviewed journals. More than 80% of these publications belong to the first quartil of impact in the field, thus showing the quality and quantity of the fundamental science produced in the Center. In spite of the fundamental nature of the Center, cooperation with industry is an important aspect that CFM pays close attention to. Several spin-off initiatives have been launched in the research lines of CFM, and during 2016 the activity of technological transfer has been explored through projects of the Department of Industry of the Basque Government, as well as with companies like Petronor who awarded CFM with one of the Inspire projects in May 2016.

In addition to the involvement of CFM staff in the Master in Nanoscience of the University of the Basque Country (UPV/EHU), the activities involving scientific outreach to the general public have gained importance, thus the increased effort at CFM towards scientific divulgation. Several activities, such as *Urban Zientzia, Mestizajes*, Week of Science, or *Fotciencia13* have been triggered out by CSIC and UPV/EHU, and have counted on CFM as a key partner during 2016.

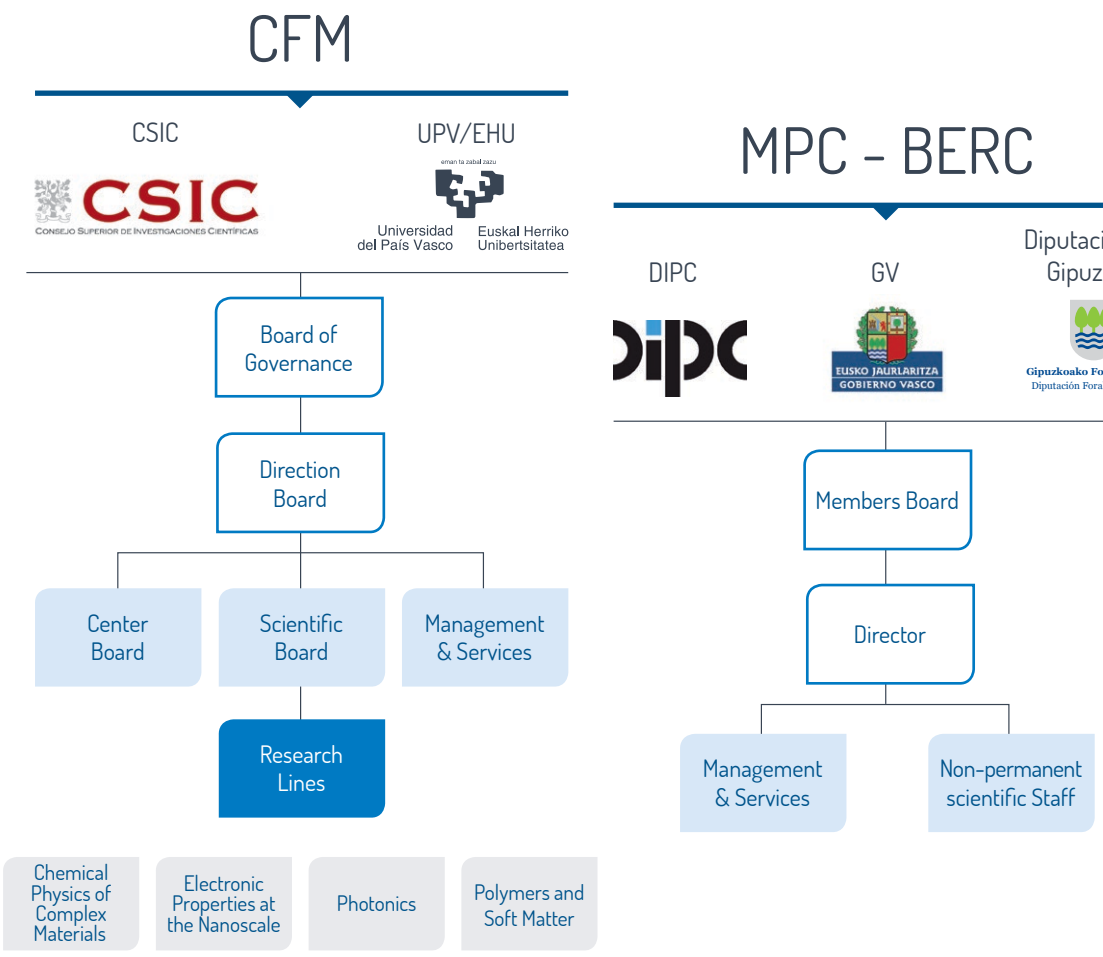
Thanks to the constant effort of the whole human team, CFM keeps its position at the forefront of research in materials science, and new and exciting challenges can now be faced in this combined effort of CSIC, the University of the Basque Country and the Basque Government. The challenge of excellence in Science is global and very competitive nowadays, and CFM is locating itself to face it with the best human and technical resources as possible.


GOVERNA

GOVERNANCE

Centro de Física de Materiales (CFM) is a joint Center of the *Spanish Consejo Superior de Investigaciones Científicas* (CSIC) and the University of the Basque Country (UPV/EHU). The main Board of Governance of the Center is constituted by the Governing Board where representatives from both CSIC and UPV/EHU designate a Direction Board which runs the daily administrative and scientific strategy of the Center. To that end the Direction board is supported by the Center Board and the Scientific Board.

The Association **"Materials Physics Center" MPC** is a non-profit association declared as Basque Excellence Research Center (BERC) which is intrinsically united to, and shares goals and scientific activity with CFM, serving as an instrumental body of activity in a totally synergistic and combined activity. The body of governance of the BERC MPC is constituted by the Basque Government (GV), the Gipuzkoa Province Government (*Gipuzkoako Foru Aldundia*), and the Donostia International Physics Center (DIPC), who appoint the scientific director of the association. The combined and united strategic activity of both CFM-MPC is ensured by the joint appointment of the same person as director of both institutional bodies.



PROFILE

Scientific staff

Research groups **14**

Researchers in action **103**

Researchers from **21** countries

31 Post-docs

33 PhD Theses on going

52 Visitors

35 Senior scientists

04 Fellows (Ikerbasque)

Training

PhD Theses defended **12**

Master theses **5**

Research Output

Isi publications **211***

Average impact factor **6,497**

H index **99**

Q1 publications **178***

Citations* **9473**

** Source Web of Science Core Collection- CFM´s ResearcherID F-4867-2012 as of April 2017*

Activities and events

Seminars **12**

Workshops **15**

Visitors from high schools **362**

Outreach activities **11**

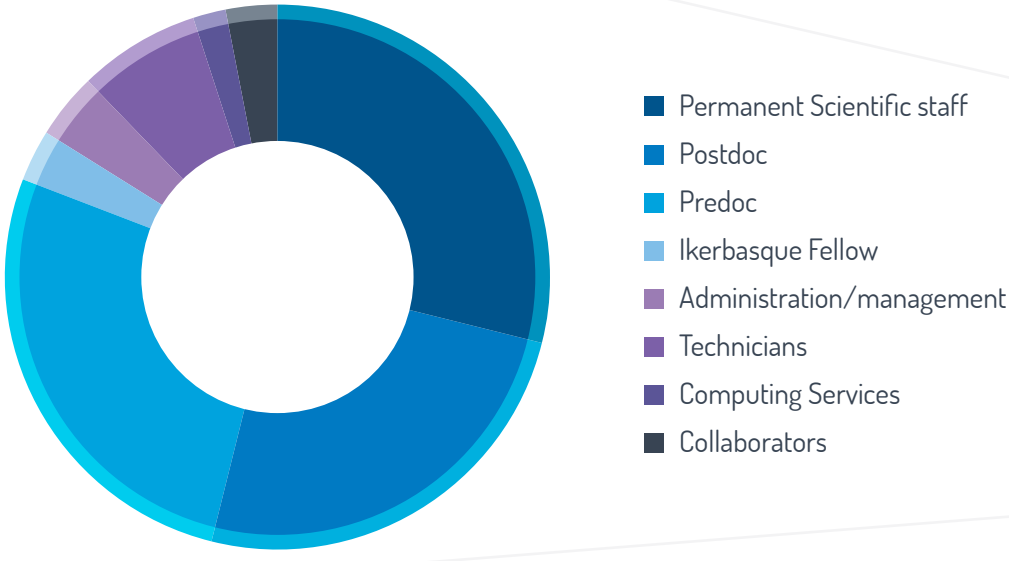
Projects and funding

38 Ongoing projects

2.186.524€ Funding 2016

PEOPLE

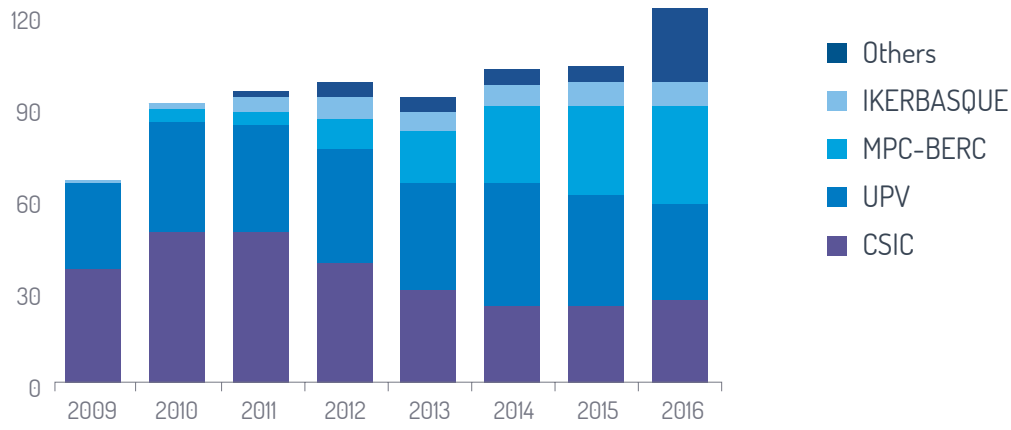
Permanent Scientific staff	35
Postdoc	31
Predoc	33
Ikerbasque Fellow	4
Administration/management	5
Technicians	8
Computing Services	2
Collaborators	4
Total	**122**



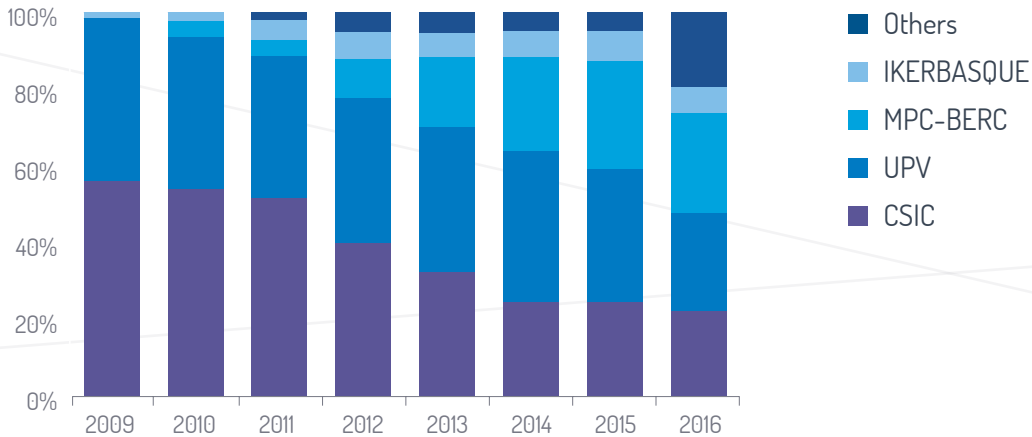
Distribution of CFM staff during 2016 according to their activity.

	2009	2010	2011	2012	2013	2014	2015	**2016**
CSIC	37	49	49	39	30	25	25	**27**
UPV	28	36	35	37	35	40	36	**31**
MPC-BERC	0	4	4	10	17	25	29	**32**
IKERBASQUE	1	2	5	7	6	7	8	**8**
OTHER	0	0	2	5	5	5	5	**24***
Total	66	91	95	98	93	102	103	**122**

**From 2016 on, we are including permanent collaborators joining CFM´s staff at the Center premises during most of the year, even if they are supported by other institutions.*



Distribution of staff at CFM in absolute numbers according to their origin through the last years.



Distribution of staff at CFM in percentage according to their origin through the years.

DIRECTION BOARD

Javier Aizpurua Iriazabal, Director
Andrés Arnau Pino, Vicedirector
Amaya Moral Arce, General Manager

MANAGEMENT

María Formoso Ferreiro, Administrative, MPC
Francisco López Gejo, Project Manager, MPC
Amaya Moral Arce, Administration Manager, CSIC
Txema Ramos Fernández, Administrative, CSIC
Jasone Ugarte García de Andoin, Executive Secretary, UPV/EHU

COMPUTING SERVICES

Garbiñe Egaña Cruz, IT Systems Technician, MPC
Iñigo Aldazabal Mensa, Computer Center Manager, CSIC

Beñat Jimenez Urbieta (Undergraduate student)

TECHNICAL SUPPORT

Silvia Arrese-Igor Irigoyen, Technician R+D+I, CSIC
María Isabel Asenjo Sanz, Technician, MPC
Luis Botana Salgueiros, Technician R+D+I, CSIC
Amaia Iturrospe Ibarra, Technician, MPC
Juan José Gil Miranda, Technitian, CSIC
Tamara Molina Rola, Student, MPC
Juan Manuel Burgos Jiménez, Technician, MPC

RESEARCHERS

Research line:

CHEMICAL PHYSICS OF COMPLEX MATERIALS

01 Gas/Solid Interfaces group

Staff

Maite Alducin Ochoa, Tenured Scientist, CSIC
Ricardo Díez Muiño, Scientific Researcher, CSIC
Iñaki Juaristi Oliden, Associate Professor, UPV/EHU

Postdoctoral Researchers

Natalia Koval

PhD Students

Oihana Galparsoro Larraza
Ivor Lončaric
Flavio Matias Da Silva
Ahmed Mohamed Abdel Azim Nosir

02 Ivo Souza Research group

Staff

Ivo Souza, Ikerbasque Professor, UPV/EHU

Postdoctoral Researchers

Stepan Tsirkin
Pablo Aguado Puente
Daniel Gosálbez

03 Nanophysics laboratory

Staff

Enrique Ortega Conejero, University Professor, UPV/EHU
Celia Rogero Blanco, Tenured Scientist, CSIC
Frederik Michael Schiller, Tenured Scientist, CSIC

Ikerbasque Fellows

Martina Corso, UPV/EHU
Sara Barja Martinez, UPV/EHU

Postdoctoral Researchers

Jens Brede
Maxim Ilin
Ruben González Moreno
Guillaume Vasseur
Luis Alejandro Miccio

PhD Students

Mikel Abadía Gutiérrez
Ignacio Piquero Zulaica

Undergraduate Student

Alberto Hijano Mendizabal

04 Modelization and Simulation group

Staff

Andrés Arnau Pino, University Professor, UPV/EHU
Daniel Sánchez Portal, Scientific Researcher, CSIC

Ikerbasque Fellow

Fernando Delgado, UPV/EHU

Postdoctoral Researchers

Pedro Brandimarte Mendonça
Mads Engelund

PhD Students

Marc Barbry
Iker Gallardo Arrieta
Federico Marchesin
Moritz mueller

05 Group of Spectroscopy at Atomic Scale

Staff

Lucia Vitali, Ikerbasque Professor, UPV/EHU

PhD Students

Ana Barragán Duran
Alexander Correa

Research line:

ELECTRONIC PROPERTIES AT THE NANOSCALE

06 Electronic Excitations in Surfaces and Nanostructures group

Staff

Andrés Ayuela Fernández, Scientific Researcher, CSIC
Pedro Miguel Echenique Landiribar, University Professor, UPV/EHU
Evgeni V. Tchoulkov, University Professor, UPV/EHU

Postdoctoral Researchers

Jhon Wilfer González Salazar
Ilya Nechaev
Marta Pelc

PhD Students

Tomás Alonso Lanza

07 Materials Computation Theory group

Staff

Aitor Bergara Jauregi, Associated Professor, UPV/EHU
José Maria Pitarke de la Torre, University Professor, UPV/EHU

PhD Students

Unai Aseguinolaza Aguirreche
Miguel Borinaga Treviño

08 Mesoscopic Physics group

Staff

F. Sebastián Bergeret Sbarbaro, Tenured Scientist, CSIC

Ikerbasque Fellow

Vitaly Golovach, UPV/EHU

Postdoctoral Researchers

Francois Xabier Konschelle
Tineke Van Den

PhD Students

Alba Pascual Gil
Cristina Sanz Fernandez

09 Nanobiospectroscopy Group

Staff

Ángel Rubio Secades, University Professor, UPV/EHU

Postdoctoral Researchers

Ali Abedi
Hannes Simon Hübener
Elham Khosravi

10 Quantum Phenomena on Surfaces group

Staff

Nicolas Lorente Palacios, Scientific Researcher, CSIC

Research line:

PHOTONICS

11 Theory of Nanophotonics group

Staff

Javier Aizpurua Iriazabal, Research Professor, CSIC
Alberto Rivacoba Ochoa, University Professor, UPV/EHU
Nerea Zabala Unzalu, Associate Professor, UPV/EHU

Postdoctoral Researchers

Yao Zhang
Mario Zapata

PhD Students

Garikoitz Aguirregabiria Achutegi
Andrea Konecna
Tomas Neuman

12 Nanomaterials and Spectroscopy group

Staff

Yury Rakovich, Ikerbasque Professor, UPV/EHU

Postdoctoral Researcher

Thomas Hendel

13 Laser Physics and Photonic Materials group

Staff

Rolindes Balda de la Cruz, University Professor, UPV/EHU
Joaquín Fernández Rodríguez, Emeritus University Professor, UPV/EHU

Research line:

POLYMERS AND SOFT MATTER

14 Polymers and Soft Matter group

Staff

Ángel Alegría Loinaz, University Professor, UPV/EHU
Fernando Alvarez González, Associate Professor, UPV/EHU
Arantxa Arbe Méndez, Research Professor, CSIC
Daniele Cangialosi, Tenured Scientist, CSIC
Silvina Cerveny Murcia, Tenured Scientist, CSIC
Juan Colmenero de León, University Professor, UPV/EHU
Angel Moreno Segurado, Tenured Scientist, CSIC
Josetxo Pomposo Alonso, Ikerbasque Professor, UPV/EHU
Gustavo Ariel Schwartz Pomeraniec, Tenured Scientist, CSIC

Postdoctoral Researchers

Petra Bacova
Edurne Gonzalez Gándara

Guido Goracci
Paula Angela Malo de Molina Hernández
Ana Lucia Rodríguez Garraza
Federica Lo Verso
Daniel Enrique Martínez Tong

PhD Students

Izaskun Letizia Combarro Palacios
Maud Formanek
Thomas Gambino
Marina González Burgos
Natalia Gutiérrez Pérez de Eulate
Stefan Holler
Alejandro Latorre Sánchez
Gerardo Martínez Rugeiro
Jon Rubio Cervilla
Jordan Ochs
Lucia Ortega Álvarez

OTHER POSITIONS

Staff

Isabel Tellería Echeverria, Associate Professor, UPV/EHU
Juan José del Val Altuna, Associate Professor, UPV/EHU

Guest Researchers

Dimas García de Oteyza, Ikerbasque Research Professor, DIPC
Fabian Barroso, Ikerbasque Research Professor, DIPC

Postdoctoral Researchers

Pawel Nita (Dimas Garcia de Oteyza´s group)

PhD Students

Nestor Merino Diez (Dimas Garcia de Oteyza´s group)

Visitors

CFM received 52 visiting researchers during 2016


EXTERNA
ADVISOR
COMMIT

EXTERNAL ADVISORY COMMITTEE

EXTERNAL ADVISORY COMMITTEE

During 2016 an External Advisory Committee was appointed at CFM-MPC. The board of members of MPC-BERC approved this appointment in the annual meeting in June 2016, and The Rector Board of CFM approved it in the ordinary session of October 2016.

The committee is formed by four renowned experts in the field of Materials Physics with knowledge and international expertise in the four research lines of the Center. These are the members of the CFM-MPC External Advisory Committee:

Institut für Chemie,
Universität Potsdam, Germany

Chair of Theoretical Chemistry,
Universität Potsdam (2008-2010)

Professor Peter Saalfrank

- **Expertise in the line at CFM:** Chemical Physics of Complex Materials
- **Merits:** Elected 'Fachkollegiat' (Referee Board Member) of Deutsche Forschungsgemeinschaft (German Research Council, DFG), "Fachkollegium Festkörper-und Oberflächenchemie: Theorie und Modellierung" (Solid State and Surface Chemistry: Theory and Modelling) (2004-2008, 2016-2019)
- **Research Interest:** Theoretical Surface Science, System-bath quantum dynamics, Laser-driven electron dynamics, Theoretical photophysics and chemistry, Electronic structure theory
- **Publications:** More than 175 ISI papers

- Often visitor of the DIPC and CFM.

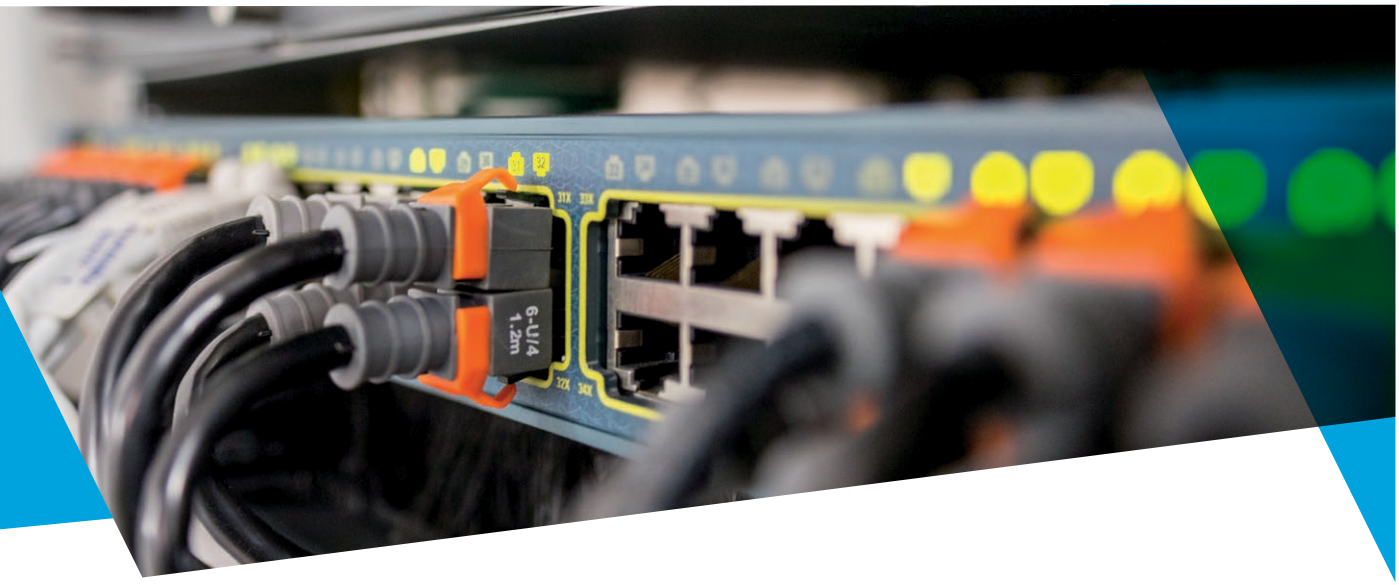
Professor Antonio Hernando Grande

- **Expertise in the line at CFM:** Electronic Properties at the Nanoscale
- **Awards:** "Académico Numerario de la Real Academia de Ciencias Exactas, Físicas y Naturales"; Doctor Honoris Causa by the UPV/EHU; Gold Medal by the "Real Sociedad Española de Física"; "Miguel Catalán" research award by the Autonomous Community of Madrid; Fellow of the American Physical Society; "Dupont" science award; "Juan de la Cierva" national research award; Doctor Honoris Causa by the "Universidad de Cantabria"
- **Research Interest:** Magnetism and related areas. He combines basic research of magnetic materials with projects in applied research
- **Publications & Patents:** More than 300 papers in ISI journals with more than 10,000 citations. Author of 20 patents

- Often visitor of the DIPC, the CFM and the UPV/EHU.

Universidad Complutense de Madrid, Spain

Director of "Instituto de Magnetismo Aplicado" (IMA)



Department of Theoretical Condensed Matter,
Universidad Autónoma de Madrid, Spain

Director of the IFIMAC- Condensed Matter Physics Center "María de Maeztu Center"

Professor Francisco J. García Vidal

- **Expertise in the line at CFM:** Photonics
- Prof. García Vidal is one of the most prestigious researchers in Photonics in the world. He knows well the reality of research in Spain, and the local boundaries for science and technology, particularly the evaluation systems in both CSIC and the ministry.
- **Research Interest:** Photonics, Nanophotonics
- **Publications:** More than 280 ISI papers
- Often visitor of the DIPC and CFM.

Professor Dr. Dieter Richter

- **Expertise in the line at CFM:** Polymers and Soft Matter
- Honors Chair at the Materials Physics Department of the University of the Basque Country founded by the Bank of Bilbao Vizcaya (1997)
- **Awards:** "Staudinger-Durrer Prize of the ETH" (2015); "Walter Hälg Prize" of the European Neutron Scattering Association (2009); "Erwin-Schrödinger Award" (2002); "Max-Planck Award" (1990) among others.
- **Research Interest:** Structure and Dynamics of Polymers and Soft Matter; Neutron Techniques and Instrumentation.
- **Publications:** More than 450 ISI papers
- Often visitor of the DIPC and CFM.

Jülich Center for Neutron Science (JNSC) and Institute of Complex Systems, Jülich, Germany

Director of the Institute for Neutron Scattering at the FZJ (1989-2014)


RESEARCH LINE
RESEARCH GRO
AND THEIR HIGH

RESEARCH LINES, RESEARCH GROUPS AND THEIR HIGHLIGHTS

RESEARCH LINES, RESEARCH GROUPS AND THEIR HIGHLIGHTS

At CFM, research activities are grouped along four main research lines, although the structure remains fully horizontal, actively seeking cross-linked, multidisciplinary research. Within the research lines, 14 recognized groups develop their activity devoted to different aspects of fundamental and applied research on the Physics of Materials.

CHEMICAL PHYSICS OF COMPLEX MATERIALS

01. Gas/Solid Interfaces group
02. Ivo Souza Research group
03. Nanophysics laboratory
04. Modelization and Simulation group
05. Group of Spectroscopy at Atomic scale

ELECTRONIC PROPERTIES AT THE NANOSCALE

06. Electronic Excitations in Surfaces and Nanoestructures group
07. Materials Computation Theory group
08. Mesoscopic Physics group
09. Nanobiospectroscopy group
10. Quantum Phenomena on Surfaces group

PHOTONIC

11. Theory of Nanophotonics group
12. Nanomaterials and Spectroscopy group
13. Laser Physics and Photonic Materials group

POLYMERS AND SOFT MATTER

14. Polymers and Soft Matter group

Chemical physics of complex materials

The research line on **"Chemical Physics of Complex Materials"** addresses the structural and electronic properties of complex nanostructured materials. Experimental and theoretical effort is combined to understand the properties, formation, and dynamics of different molecules and nanostructures at surfaces.

Five research groups are included in this research line, with a high degree of complementarities. Three of the groups devote their activity to the ab-initio theoretical study of electronic structure and dynamical processes of nanostructures and molecules in the proximity of surfaces, as well as to condensed matter states which show interesting topological properties. These groups are the "Gas/Solid Interface Group", the "Modelization and Simulation Group", and the "Ivo Souza's Group". Two of the groups in this research line develop experimental activity on the electronic properties of molecules and low dimensional structures, which are studied with the use of Scanning Tunneling Microscopy (STM) techniques at ultrahigh vacuum and low temperature. These groups are the "Nanophysics Laboratory" and the "Group of Spectroscopy at the Atomic Scale".

01

GAS/SOLID INTERFACES GROUP

In general terms, understanding and mastering the physics and chemistry of adsorption processes at nanostructures and surfaces is a basic requirement for the full development of nanoscience and nano-technology. Metal surfaces are effective chemical agents capable of adsorbing and/or dissociating molecules impinging from the gas phase. Industrial processes of enormous economical impact, such as corrosion and heterogeneous catalysis, greatly benefit from recent developments in basic research on this matter. Over the last years, the combination of experimental molecular-beam techniques and refined theoretical calculations based on ab-initio methods have led research on the field to a new stage, in which detailed investigations of the kinetics and dynamics of molecular reactivity at surfaces are possible.

The "Gas/Solid Interfaces" group is mainly interested in the elementary reactive processes that may happen whenever atoms or small molecules interact with surfaces. When a molecule approaches the surface, intramolecular chemical bonds can break down and new ones can be formed with the surface. The group uses first-principles electronic structure calculations to describe the details of the interaction between the incoming species and the surface through a multidimensional potential energy surface (PES). Once the PES of the system is known, they simulate the dynamics of several processes by solving the classical equations of motion of the nuclei.

Particular attention is paid to non-adiabatic processes and the energy dissipation channels that come into play, because they can drastically change the output of the dynamics. From a theoretical point of view, the description of ground state properties is currently well founded and has proven to be extremely successful in explaining elementary reactive and non-reactive adiabatic processes at surfaces. The description of excited states and the evaluation of energy transfer mechanisms is however still maturing and further developments are needed to reach the same level of detail in the understanding and of accuracy in the quantitative representation.

Group Leader: Ricardo Diez Muiño, Scientific Researcher, CSIC

HIGHLIGHT

Surface electron density models for accurate ab initio molecular dynamics with electronic friction

Novko D, Blanco-Rey M, Alducin M and Juaristi JI.

Physical Review B 93, 245435 (2016)

The interaction of thermal atoms and molecules with surfaces and nanostructures are ever-present in our daily life as well as in many industrial applications. The oxidation and corrosion of surfaces, the catalytic converters used in cars, or the industrial production of most synthetic compounds are relevant examples of the importance of the elementary reaction processes arising in gas/surface interfaces. Within this context, the challenge in present computational surface science is to count with reliable theoretical models that can predict the outcome of a specific reaction.

In the last decade, the ever more powerful computational resources have permitted us to advance in our understanding of gas-surface reactivity from first principles. There are many theoretical studies confirming that the fundamental properties in most elementary gas-surface processes are satisfactorily described by the Born-Oppenheimer approximation, which neglects the coupling between electronic excitations and the nuclear motion. Still, the challenge in present gas-surface simulations is to provide a reliable description of the two main energy exchange channels that may affect the dynamics and reactivity of atoms and molecules on solid surfaces, namely, phonons and electron-hole (e-h) pair excitations. In the end, these are the mechanisms that dictate, on the one side, the thermalization rate and, hence, the mean traveled length of the nascent adsorbates, and, on the other side, the mean traveled path of the desorbing species. It is the balance between all these key quantities that will determine the catalytic properties of the surface.

In order to tackle this issue, the gas-surface dynamics group at CFM has developed the so-called ab initio molecular dynamics with electronic friction (AIMDEF) scheme that provides a joint and reliable description of the effect that e-h pairs and phonons will have on elementary reactions at metals. Using this new AIMDEF method to study the relaxation dynamics of different atoms and molecules, the authors are able to extract general trends on the role and competition between both energy exchange channels: (i) e-h pairs are expected to dominate the dynamics of light gas species and (ii) even if phonons will increasingly dominate the heavier hot species, the contribution of e-h pairs is by no means negligible in these cases because it gains relevance at the last stage of the relaxation process.

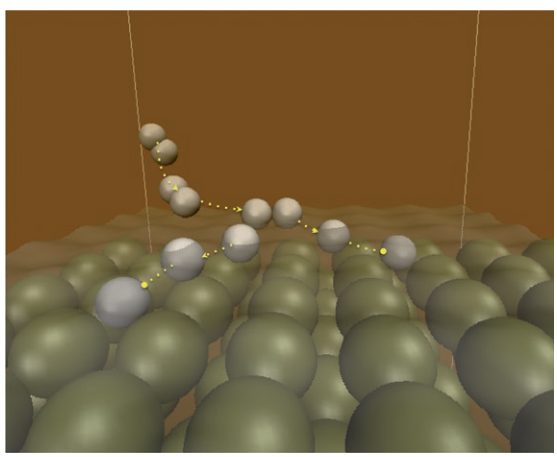


Figure: Schematic representation of electron-hole pair excitations during the dissociative adsorption of H_2 on Pd(100)

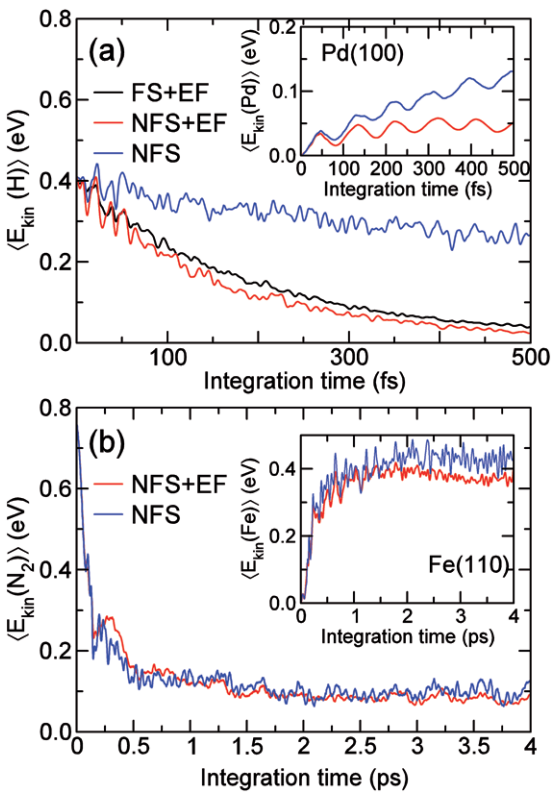


Figure: (a) Time evolution of the mean kinetic energy of the nascent H atoms formed upon dissociation of 0.5 eV H_2 on Pd(100). (b) Same for 0.75~eV N_2 adsorbing on Fe(110). Results obtained from different AIMDEF simulations: including both e-h pairs and phonons (red curves, labeled NFS+EF), only phonons (blue curves, labeled NFS), and only e-h pairs (black curve, labeled FS+EF). Each inset shows the mean kinetic energy of the surface atoms versus time.

02

IVO SOUZA RESEARCH GROUP

"Ivo Souza research" group activity is focused into condensed-matter theory, using computational techniques to study the properties of materials from first-principles. The group's work often involves the development of new theoretical approaches and algorithms, and their application to problems of current interest, including methods to study insulators in finite electric field, as well as to construct localized Wannier orbitals for metals. Phenomena which arise from the interplay between the collective magnetic order in solids and the spin-orbit interaction inside the constituent atoms have been recently addressed as well.

The group has introduced methods to study insulators in finite electric fields, and to construct localized Wannier orbitals for metals. Currently the ground-state and transport phenomena that arise from broken symmetries such as time reversal (magnetic order) and spatial inversion is being studied. Examples include the anomalous Hall effect and orbital magnetization in ferromagnetic metals, the valley Hall effect in transition-metal dichalcogenides, and magnetoelectric effects in topological insulators, magnetic oxides, and gyrotropic metals. A recurring theme in Ivo Souza´s research is the use of geometric phases and related concepts (Berry curvature, Chern number, intrinsic orbital moment) to describe the electronic properties of solids.

Group Leader: Ivo Souza; Ikerbasque Research Professor, UPV/EHU

HIGHLIGHT

Gyrotropic Magnetic Effect and the Magnetic Moment on the Fermi Surface

Zhong SD, Moore JE and Souza I.

Physical Review Letters 116, 7 (2016)

Optical responses in chiral topological semimetals

One of the characteristic signatures of topological phases is the existence of robust gapless states in the surface band structure. In addition, topological phases that are insulating in the bulk often have quantized bulk electromagnetic responses, such as the integer quantum Hall effect. Gapless phases with topological features, such as Dirac and Weyl semimetals in 3D, can also have interesting electromagnetic responses, although one might not expect them to be quantized. In this work this group found that certain nonmagnetic Weyl semimetals display a peculiar type of magnetoelectric effect: a bulk current is induced by an oscillating magnetic field and, conversely, a bulk magnetization is induced by the passage of a current. This "kinetic magnetoelectric effect" is the low-frequency limit of natural optical activity, and it should be observable in optical rotation on mirror-free Weyl semimetals. Microscopically, it is determined at low frequency by the magnetic moments of Bloch electrons on the Fermi surface. While the effect is not exclusive to Weyl semimetals, for them it takes a particularly simple form: the rotatory power is proportional to the energy separation between the 3D bulk Dirac cones of opposite chirality.

At present the group is using first-principles methods to investigate this and related optical phenomena (e.g., the current-induced Faraday rotation) in chiral nonmagnetic conductors such as doped trigonal tellurium. In this material, the Te atoms form helical chains, as depicted in the figure. The passage of a current along the helical axis then induces a parallel orbital magnetization, i.e., it is as if the helical chains behaved like microscopic solenoids.

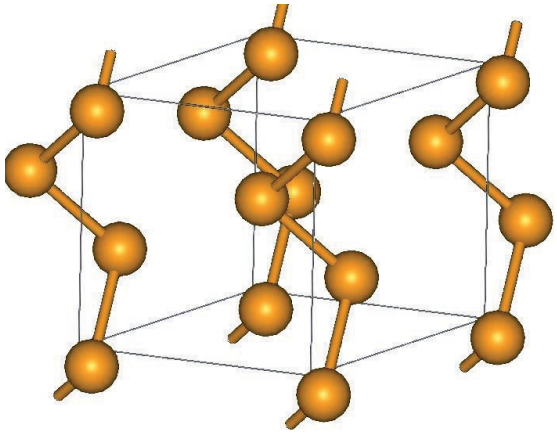


Figure: The crystal structure of trigonal tellurium. The tellurium atoms are arranged along helical chains, which can be either right-handed (as shown here) or left handed.

Group Leader: Enrique Ortega, University Professor, UPV/EHU

03 NANOPHYSICS LABORATORY

The research activity of this group focuses on the morphology and the electronic states in a diversity of nanostructures and low dimensional objects, following the Surface Science approach, namely Ultra-High-Vacuum (UHV) and in-situ (vacuum) substrate preparation and Molecular Beam (MBE) epitaxy. The main experimental techniques include Angle-resolved Photoemission Spectrocopy (ARPES), X-ray Photoemission Spectroscopy (XPS), Magneto-Optic Kerr Effect (MOKE), and Scanning Tunneling Microscopy/Spectroscopy (STM/STS). Photoemissions, as well as Near Edge X-ray Absorption (NEXAFS) experiments are also carried out at different Synchrotron radiation facilities around the world: ALS in Berkeley, Elettra in Trieste, Soleil in Paris, Max-Lab in Lund, and the SLS in Zurich.

HIGHLIGHT

Interplay between Steps and Oxygen Vacancies on Curved TiO2(110)

Miccio LA, Setvin M, Muller M, Abadia M, Piquero I, Lobo-Checa J, Schiller F, Rogero C, Schmid M, Sanchez-Portal D, Diebold U and Ortega JE.

Nano Letters 16, 2017 (2016)

Rutile is the most stable polymorph of titanium dioxide (*r*-TiO_2), being a prototypical, reducible metal oxide. It is applied in many fields ranging from catalysis to memristors. These applications are often enabled by lattice defects, which act as electron donors and convert the otherwise insulating system into an *n*-type semiconductor. The nature of these defects, as well as their influence on the electronic and chemical behavior of *r*-TiO_2, has attracted considerable interest. Of particular importance are oxygen vacancies, which donate electrons to the material. Excess electrons in rutile tend to localize at surface and subsurface Ti atoms, forming a Ti^{3+} oxidation state. The localized electron is accompanied by lattice distortions, leading to the so-called polaron of *r*-TiO_2.

Step edges are sites with low atomic coordination and thus chemically and electronically active. Only a few studies on vicinal rutile planes exist, but they reveal the potential of stepped surfaces to further tailor the physical and chemical properties of *r*-TiO_2. However, a systematic study of different vicinal planes exploring their structural stability, the step edge termination, the contributions of steps to electron-doping, or the possible alteration of the Ti^{3+} polaron in the vicinity of steps, is missing. In this work we demonstrate that a thorough exploration of structural and electronic properties of stepped *r*-TiO_2(110) surfaces can be conveniently performed using curved crystals.

In the figure bellow (a) the photography of the curved TiO_2(110) sample (c-TiO_2(110)), which allowed the systematic study of stepped *r*-TiO_2(110) surfaces with tunable density of [1-10]-oriented steps is shown. Using Scanning Tunneling Microscopy we analyzed the structure and distribution of steps and vacancies as a function of the average deviation (miscut α) from the (110) surface. A smooth evolution from wide terraces, containing oxygen bridge vacancies is observed [O_{br} vac´s, Figure (b)], toward narrow (110) terraces, depleted of O_{br} vac´s, but exhibiting a high density of triangularly-shaped protrusions at steps (S_t) [Figure (c)]. By scanning the photoemission beam in angle resolved photoemission spectroscopy across the sample, we studied the signature of the Ti^{3+} polaron, namely the so-called Ti^{3+} gap state [Figure (d)]. The gap state reflects a transition from O_{br} to step-edge-doping across the curved surface through a 110 meV shift in apparent binding energy, indicating a different polaronic relaxation for flat or stepped surfaces. Interestingly, the intensity of the gap state correlates with the sum of O_{br} vac´s at terraces and S_t step-protrusions, suggesting that every S_t site hides one oxygen vacancy that equally contributes to sample doping in *r*-TiO_2(110).

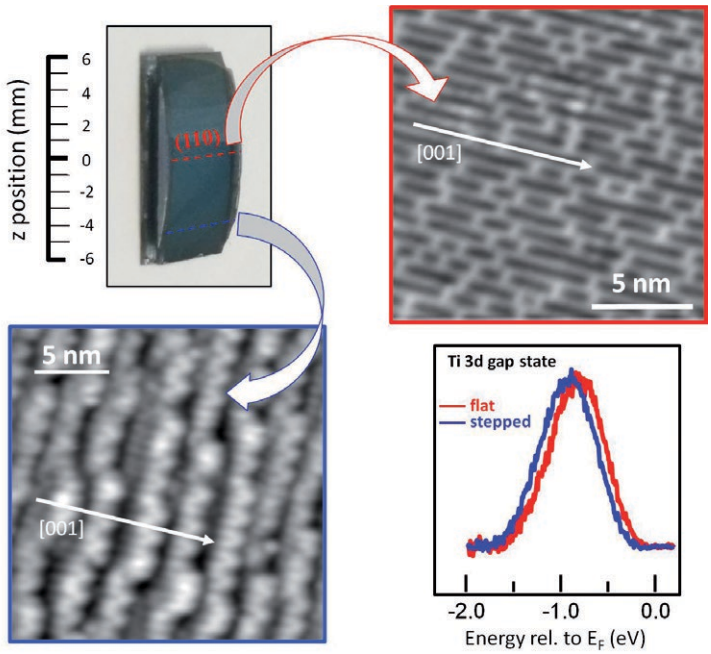
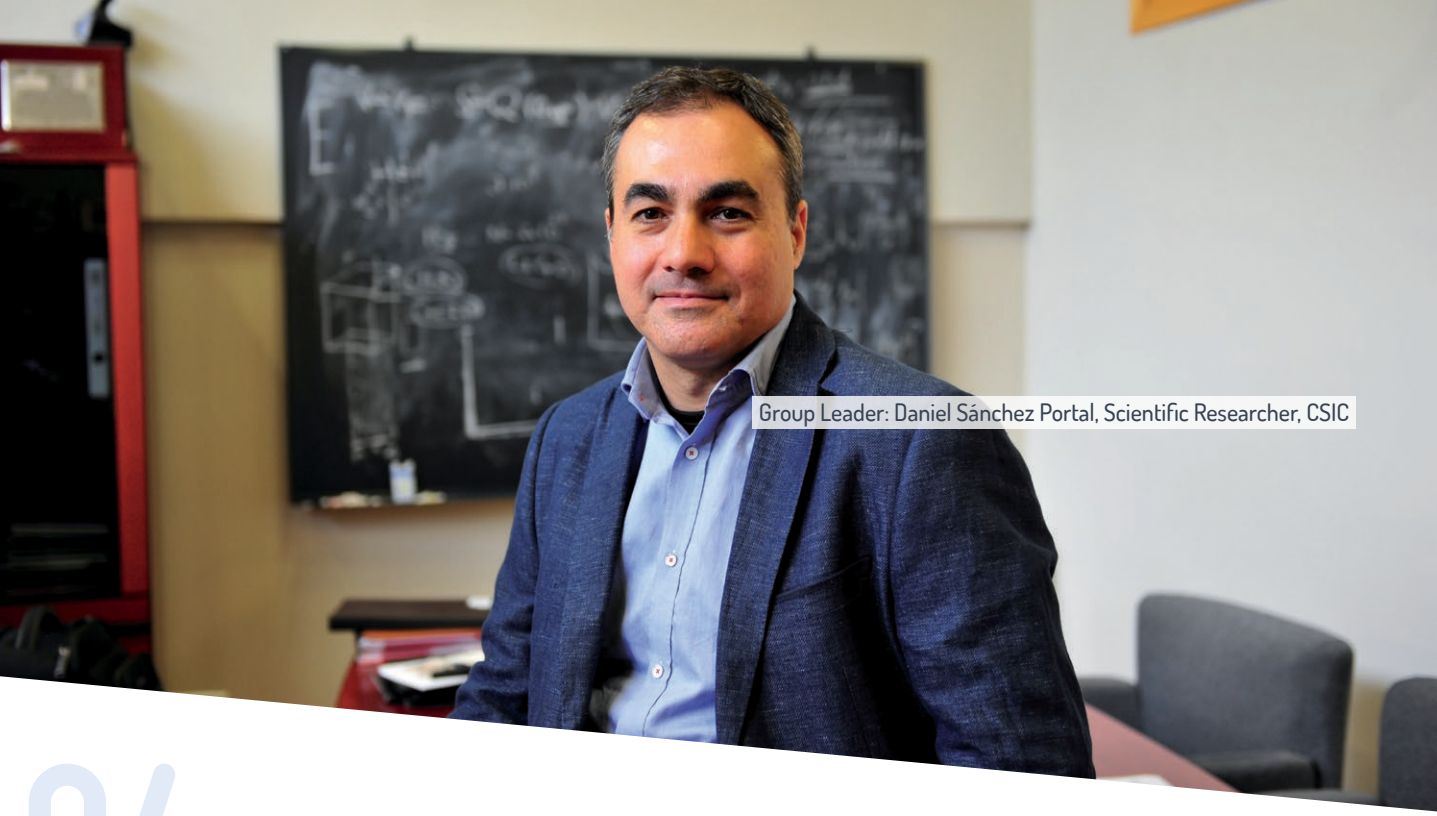


Figure: (a) Curved TiO_2(110) sample. The (110) plane is located at the center of the curved crystal, and the step density smoothly increases towards both sides. Marked are the positions at which the Scanning Tunneling Microscopy images (b)-(c) were obtained. (b) (110) terrace with O_{br} vac´s appearing as bright, features bridging bright Ti rows along the (001) direction. (c) Narrow O_{br} vac´s-free terraces, regularly separated by [1-10]-oriented steps. The latter feature triangularly-shaped St protrusions (bright features). (d) Gap state peak measured from flat [panel (b), red line] and stepped [panel (c), blue line] areas of the curved crystal, using Angle Resolved Photoemission. The intensity is exactly the same, meaning that each S_t site hides one oxygen vacancy that dopes the stepped TiO_2(110) surface.



Group Leader: Daniel Sánchez Portal, Scientific Researcher, CSIC

04 MODELIZATION AND SIMULATION GROUP

The "Modelization and Simulation" group is devoted to the theoretical study of the electronic and structural properties of complex materials, clean and decorated surfaces, and nanostructures, by using first-principles methods. An important part of the research activity is devoted to the development of simulation tools. This group is one of the teams involved in the development of the linear-scaling SIESTA code for ab-initio calculations. Other research areas of the group include: first-principles simulations of elastic and inelastic transport in nanostructures; simulations of scanning tunneling microscopy images and tunneling spectroscopies; theory of the interaction of ions and fast particles with solids, surfaces and nanostuctures; ultra-fast electron processes and electronic excitations.

HIGHLIGHT

Quantum Transport Revealed in Optics: Plasmonic Response of Metallic Nanojunctions Driven by Single Atom Motion

Marchesin F, Koval P, Barbry M, Aizpurua J and Sánchez-Portal D.

ACS Photonics 3, 269-277 (2016)

Can individual atoms drive Optics? This seems difficult since the wavelength of visible light is thousands of times larger than the typical atomic dimensions. However, with the promise of molecular electronic devices, closing this length-scale gap has become a key open issue in the search for novel electro-optical devices. Plasmons are known for their ability to localize light down to the nanometer scale. Unfortunately, this

is still at least one order of magnitude larger than the typical atomic size. In this communication, the group showed that the distribution of local fields around metal nanoparticles is affected by their structure at the atomic scale. However, the optical response in the far field is usually quite insensitive to such details. Thus, the question arises whether this can be done better. Can the rearrangement of a few atoms influence the plasmonic response of a nanometer-scale object in a way that can be measured by optical means?

The modelization and simulation group at CFM gives an affirmative answer to these questions. The conclusions driven by the results stem obtained from a theoretical analysis of the properties of a plasmonic cavity (see the Figure below) formed by two nanoparticles, a canonical model for tip-enhanced spectroscopy setups. These calculations are possible thanks to the efficient implementation of linear response theory within the framework of time-dependent density functional theory (TDDFT). The researchers observe the spontaneous formation of ultrathin metal necks across a metal nanojunction, which features quantized electron transport. Due to this quantization, changes of the contact cross-section involving just one atom give rise to discontinuous, abrupt changes in the current. In this work, it is demonstrated that such quantized current jumps translate into sudden changes of the intensities, spectral positions and widths of the cavity plasmon resonances. The simulations are not a mere theoretical "divertimento". Nanocontacts similar to those described in our report but made out of gold, a prototypical plasmonic material, have been already fabricated and studied in experimental laboratories worldwide.

Thus, these results indicate that the far-field optical response of nanometer-sized objects can be tuned by structural rearrangements involving a few or even a single atom, opening new avenues for research of active control devices in Nanoptics.

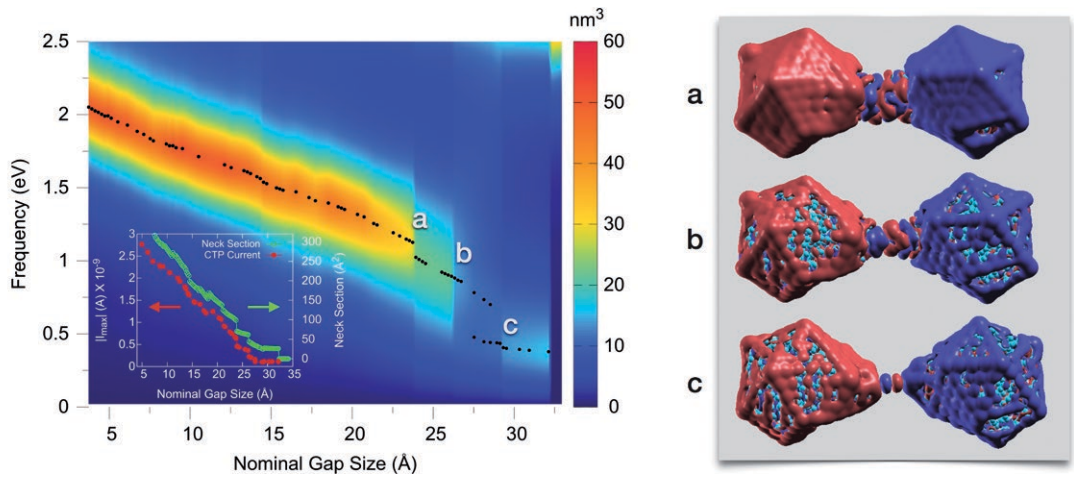


Figure: Left panel: Evolution of the resonances in the imaginary part of the polarizability as a function of the junction size. Due to the spontaneous formation of a metal neck across the nanojunction, we can observe a characteristic charge-transfer plasmon (CTP) mode all the way up to ~30 Å nominal separations between the particles. The inset shows the electric current flowing through the junction (at the frequency of the CTP resonance), and the evolution of the cross-section of the neck. There is a one-to-one correspondence between the jumps observed in the current, in the neck cross-section and in the far-field optical response of the plasmonic cavity. Right panels: Structure of the system formed by Na380 particles at the separations indicated as (a), (b) and (c) in the left panel. Imaginary part of the induced electronic charge distribution at the CTP resonance frequency for each of the configurations is also plotted (different colors indicate charge accumulation and charge depletion).

HIGHLIGHT

Ultrafast electronic response of graphene to a strong and localized electric field

E. Gruber, R. A. Wilhelm, R. Pétuya, V. Smejkal, R. Kozubek, A. Hierzanberger, B. C. Bayer, I. Aldazabal, A. K. Kazansky, F. Libisch, A. V. Krasheninnnikov, M. Schleberger, S. Facsko, A. G. Borisov, A. Arnau and F. Aumayr.

Nature Communications 7, 13948 (2016).

New experiments and simulations have shown that it is possible for extremely high currents to pass through graphene. This allows imbalances in electric charge to be rapidly rectified without introducing any damage in the graphene layer.

An international research team, formed by both theorists (CFM-UPV/EHU and DIPC, Donostia, and CNRS, Paris) and experimentalists (Helmholtz-Center, Dresden-Rossendorf, University of Duisburg-Essen and TU, Wien), was able to prove that electrons in graphene are extremely mobile and react very quickly to an ultrahigh electric field. In the experiments, xenon ions, with a particularly high electric charge, impact on a graphene single layer film producing a large number of electrons to be torn away from the graphene in a very precise spot. However, thanks to the theoretical simulations, it was possible to understand that the material is able to replace the electrons within some femtoseconds. This resulted in extremely high currents, which would not be maintained under normal circumstances. Its extraordinary electronic properties make graphene a very promising candidate for future applications in the field of electronics.

The highly charged Xe ions used in the experiments have initial positive charges up to +35, which means that 35 electrons have been removed in the ion source before it collides with the graphene film. However, as it is approaching the film it starts tearing electrons away from the graphene due to its extremely strong electric field. By the time the ion has fully passed through the graphene layer, it has a positive charge of less than +10, compared to over +30 when it started out. The ion is able to extract more than 20 electrons from a tiny area of the graphene film. This means that electrons are now missing from the graphene layer, so the carbon atoms surrounding the point of impact of the xenon ions are positively charged.

The group´s simulations using time dependent density functional theory (TDDFT) reveal the highly nonlinear multielectron processes responsible for the ultrafast response (few femtoseconds) of graphene electrons to the extremely high electric field produced by the highly charged ion. These processes take place in a few nanometers size spot of the graphene layer, something that translates into extremely high current densities both in the perpendicular and transverse directions to the graphene plane, as shown in the figure below. Additionally, the team shows that the experimentally measured keV energy loss experienced by the highly charged ion is transferred to electronic degrees of freedom. Mainly the energy is taken away by ionization of several tens of electrons into the continuum. The holes left in a nm size graphene area as a result of an electron emission and electron capture by the projectile are so quickly neutralized that there is no time to transfer the energy to the lattice producing structural defects.

This extremely high electron mobility in graphene is of great significance for a number of potential applications, like the construction of ultrafast electronic devices or connecting optical and electronic components.

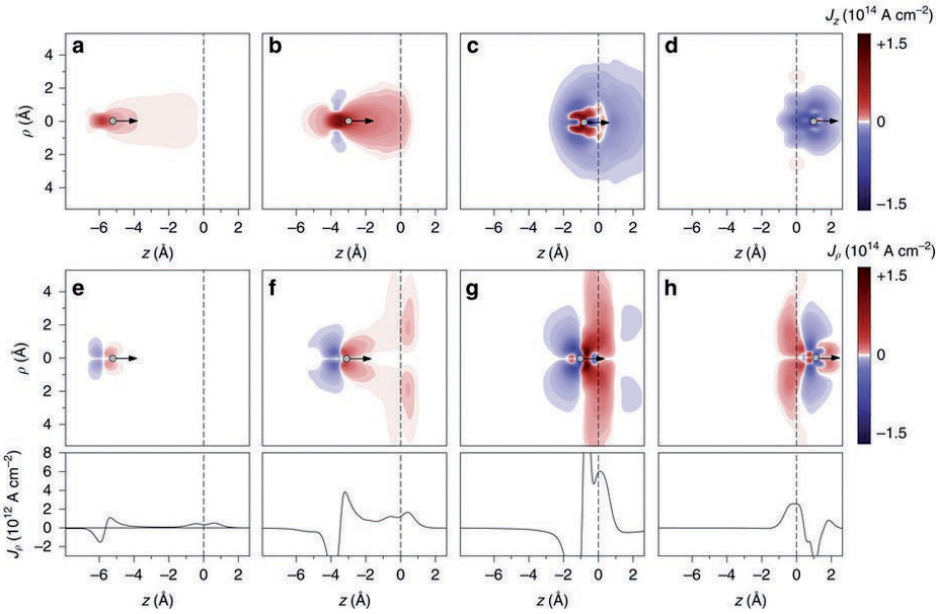


Figure: Snapshots of the perpendicular J_z (a–d) and radial J_ρ (e–h) components of the current density for q_{in}=20 at four different HCI–graphene distances obtained from TDDFT calculations performed in cylindrical (ρ,z) coordinates with z-axis set along the projectile trajectory perpendicular to the target surface. The figures show that already above the graphene layer electrons are transferred to the approaching HCI and the current density along the direction of motion explains the charge exchange of the HCI. Extremely high transverse current density (f–h) along the graphene layer is obtained. The corresponding profiles (lower panels) show the z-dependent transverse current density averaged over a circle of 10 Å in radius. Values exceeding 10^{12} A cm^{-2} are obtained. The position of the HCI is indicated by a small circle, while the position of the graphene layer by the vertical dashed line.

05

GROUP OF SPECTROSCOPY AT ATOMIC SCALE

The “Spectroscopy at the atomic scale” group is devoted to structural and spectroscopic investigations at the local scale, based on scanning tunneling techniques. Electronic, vibrational, and transport properties at surfaces are addressed. The group’s main tool for studying nanostructures at the atomic scale is low temperature scanning probe microscopy. Local properties of nanoscale objects and surfaces are thus probed in ultra-high vacuum and at temperatures down to 1K.

Group Leader: Lucia Vitali, Ikerbasque Research Professor, UPV/EHU

HIGHLIGHT

Strain-induced effects in the electronic and spin properties of a monolayer of ferromagnetic GdAg2

Correa A, Xu B, Verstraete MJ and Vitali L.

Nanoscale 8, 19148 (2016)

Geometrical structure, lattice periodicity and atomic arrangement are subtly intertwined with the electronic properties of materials. Sub-angstrom changes in the atomic distance are sufficient to modify the physical and chemical properties, such as the band-structure, carrier mobility and the chemical reactivity. This implies that considerable progress in tailoring the electronic and optical properties can be obtained by strain-engineering two dimensional layers structures. In mesoscopic systems formed by few-layers thick ferromagnetic materials, structure relaxation processes and in-plane strain lead to additional interesting effects in the magnetic properties.

In this collaborative work, carried out by the groups led by Matthieu Verstrate (University of Liege), Bin Xu (University of Arkansas) and Lucia Vitali (CFM, UPV/EHU, Ikerbasque), it has been successfully demonstrated that the electronic and magnetic properties of a monolayer of GdAg2, on Ag(111), can be modified via a thermal-controlled surface-strain of the intra-layer atomic distance, leading to lateral hetero-structuring. The GdAg2 layer, which differs in lattice constant from the supporting Ag(111), leads to the formation of a moiré superstructure. In these superstructures, the atoms of the alloy are in a periodically shifting stacking configuration with respect to the one of the supporting layer. Therefore, also the interlayer coupling varies. This induces an out-of-plane atomic buckling of the supporting substrate at a defined position of the moiré structure. This relaxation effect and the variable coupling interaction steer a modulation in the density of states and a local weakening of the ferromagnetic order resulting in a spin-texture across the layer. These results provide perspectives for control of electronic properties and magnetic ordering in atomically-thin layers.

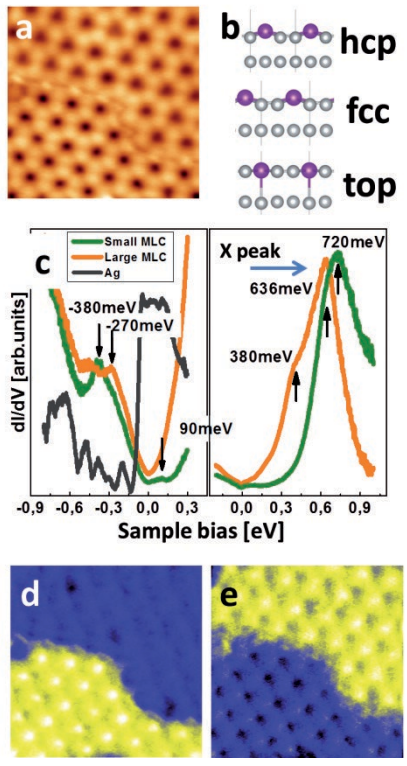


Figure: Topographic image showing a lateral-hetero-structure formed by two GdAg2 moiré superstructures differing in lattice constants. Image size 20 nm × 20 nm (b) Calculated relaxed geometry for the GdAg2/Ag(111) in three different stacking configurations (hcp, fcc and top) and inducing variable atomic relaxations. Electron density of states (c) and conductance maps (380 meV and 700 meV) (d–e), showing the localization of the electronic peaks either of the two moiré superstructures.

Electronic Properties at the Nanoscale

The research line on **"Electronic Properties at the Nanoscale"** focuses on the electronic properties of solids, surfaces, nanostructures, and low-dimensional systems. Research within the line tackles the electronic properties both of ground and excited states of these systems. In particular, the electronic response of materials under different perturbations, i.e., different experimental probes (electromagnetic radiation, electrons, ions, etc.), is investigated. The way in which size, border, and dimensionality effects can change the properties of nanosized materials is under scrutiny. Five research groups are included in this purely theoretical research line. The activity of all groups together covers the theoretical study of a wide range of materials, including both the microscopic and the mesoscopic scales, based on state-of-the-art theoretical methodologies.

06 ELECTRONIC EXCITATIONS IN SURFACES AND NANOESTRUCTURES GROUP

The "Electronic Excitations in Surfaces and Nanostructures" group is mostly devoted to the theoretical study of electron dynamics in solids, surfaces, nanoscale systems and materials of technological interest. Furthermore, electronic and magnetic properties of materials are obtained using first principles methodologies. Electron dynamics in different systems is investigated, with particular emphasis on ultrafast processes and size effects. Advanced materials, such as topological insulators and cement-related systems, are current targets of the group's research.

Group Leader: Andrés Ayuela (Scientific Researcher, CSIC)

HIGHLIGHT

Existence of nontrivial topologically protected states at grain boundaries in bilayer graphene: signatures and electrical switching

Jaskolski W, Pelc M, Chico L, Ayuela A.

Nanoscale 8, 6079 (2016)

In this work it is discovered that in gated bilayer graphene, gap states with topological origin may be present despite having stacking boundaries, which introduces atom-size defects that cause mixing between sublattices. Furthermore, the number of gap states depend on the sign of the gate voltage applied, a fact of interest for the design of future electronic devices.

The appearance of gapless states in stacking domain walls can be much more common in bilayer graphene. They are also shown in unexpected geometries, for instance at grain boundaries with atomic-scale topological defects. We focus on bilayer graphene in which one of the layers contains a line of octagon—double-pentagon defects. This work demonstrates that even with pentagonal defects mixing graphene sublattices, gap states are preserved. It is however observed that both topological and defect-originated states strongly hybridize in a game mainly determined by the gate voltage polarization. Thus, unlike previous predictions, the number of gap states changes by inverting the gate voltage sign, which originates an asymmetric conductance along the grain boundary under gate reversal. The authors expect that this effect, linked to defect states, should be detectable in transport measurements and could be exploited in electrical switches.

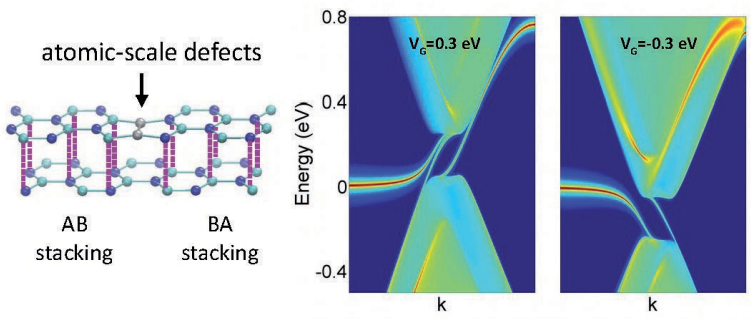


Figure: Bilayer graphene having a boundary with a change of stacking from AB to BA built by a defect line in the top layer. (a) Structural model. Atoms are colored in cyan and blue following the A and B sublattices, respectively. The nodes in grey color are mixing the two sublattices. Local density of states as a function of energy and wavevector along the defect line, for gate voltages either (c) positive V=0.3 eV or (d) negative V=-0.3 eV. Note that due to gate voltage polarization, the number of gap states is assymetric.

Group Leader: Aitor Bergara, Associate Professor, UPV/EHU

07 MATERIALS COMPUTATION THEORY GROUP

The "Materials Computation and Theory" group focuses into first-principles electronic structure calculations to analyze and understand materials properties, in particular optical, electronic and magnetic properties, as well as superconductivity. A theoretical analysis of the experimentally observed, and still not completely understood, anomalous physical properties associated to the increasing pressure induced electronic correlation are also addressed.

HIGHLIGHT

Gold as a 6p-Element in Dense Lithium Aurides

Yang GC, Wang YC, Peng F, Bergara A and Ma YM.

Journal of the American Chemical Society 138, 4046 (2016)

The negative oxidation state of gold (Au) has drawn a great attention due to its unusual valence state that induces exotic properties in its compounds, including ferroelectricity and electronic polarization. Although monatomic anionic gold (Au–) has been reported, a higher negative oxidation state of Au has not been observed yet. Here the group at CFM proposed that high pressure becomes a controllable method for

preparing high negative oxidation state of Au through its reaction with lithium. First-principles calculations in combination with swarm structural searches disclosed chemical reactions between Au and Li at high pressure, where stable Li-rich aurides with unexpected stoichiometries (e.g., Li4Au and Li5Au) emerge. These compounds exhibit intriguing structural features like Au-centered polyhedrons and a graphene-like Li sublattice, where each Au gains more than one electron donated by Li and acts as a 6p-element. The high negative oxidation state of Au has also been achieved through its reactions with other alkali metals (e.g., Cs) under pressure. This work provides a useful strategy for achieving diverse Au anions.

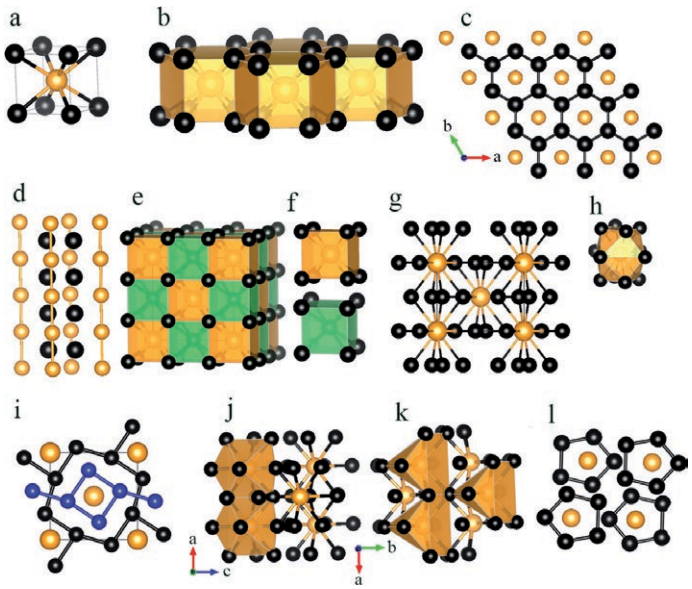


Figure: Stable structures of LinAu (n = 1–5) at 50 GPa. The lattice parameters of all of the structures are listed in the Supporting Information (Table S1). (a) LiAu in the Pm-3m structure. (b) Li2Au in the P6/mmm structure. (c) A Li graphene-like layered structure in the P6/mmm structure of Li2Au. (d) Linear Au chains in the P6/mmm structure of Li2Au. (e) Li3Au in the Fm-3m structure. (f) View of hexahedrons in Li3Au. (g) Li4Au in the I4/m structure. (h) View of a dodecahedron in Li4Au. (i) Square Li4 and octagonal Li8 rings in the I4/m structure of Li4Au. (j and k) Li5Au in the Cmcm structure. (l) Planar five-membered Li5 pentagonal rings in the Cmcm structure of Li5Au. In all the structures, small black or blue and large golden spheres represent Li and Au atoms, respectively.

08 MESOSCOPIC PHYSICS GROUP

The “Mesoscopic Physics” group is devoted to the theoretical study of the properties of mesoscopic systems, as well as to the study of quantum transport in metals, ferromagnets, semiconductors, superconductors, cold-atoms systems, organic materials and insulators. The main goal of the group is the development of theoretical frameworks to describe several phenomena related to quantum transport in mesoscopic systems, such as the coexistence of ferromagnetism and superconductivity, heat transport in nanostructures, quantum coherence in hybrid systems, and strongly correlated systems.

Group Leader: Sebastián Bergeret, Tenured Scientist, CSIC

HIGHLIGHT

The ω-SQUIPT as a tool to phase-engineering of Josephson topological materials

Strambini E, D'Ambrosio S, Vischi F, Bergeret FS, Nazarov YV and Giazotto F.

Nature Nanotechnology 11, 1055 (2016)

Multi-terminal superconducting Josephson junctions based on the proximity effect offer the opportunity to tailor non-trivial quantum states in nanoscale weak links. In collaboration between the theory groups of Sebastian Bergeret at the CFM and Yuli Nazarov at the Delft University of Technology, together with the experimental group of Francesco Giazotto in Pisa, a three-terminal Josephson interferometer has been analyzed. Tunneling spectroscopy measurements reveal transitions between gapped (that is, insulating) and gapless (conducting) states that are controlled by the phase configuration of the three superconducting leads connected to the junction. These transitions are of topological origin: a gapless state necessarily occurs between two gapped states of different topological indices, in much the same way that the interface between two insulators of different topologies is necessarily conducting. The topological numbers that characterize such gapped states are given by superconducting phase windings over the two loops that form the Josephson interferometer. As these gapped states cannot be transformed to one another continuously without passing through a gapless condition, they are topologically protected. The findings of this work are pivotal for enabling phase engineering of different and more sophisticated artificial topological materials.

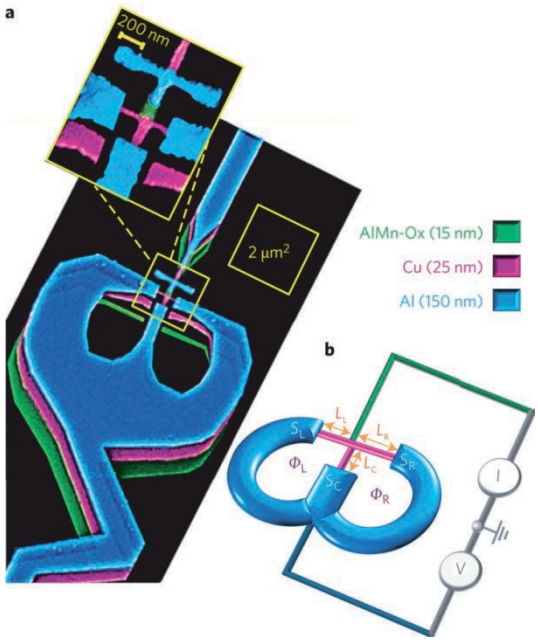


Figure: (a) False-color tilted scanning electron micrograph of a typical ω-SQUIPT. The inset highlights the core of the interferometer: a nanosized T-shaped proximised Cu weak link (magenta) in clean metallic contact with two Al superconducting loops (blue). The area of each loop is around 2μm². The central part of the weak link is tunnel-coupled to a ~100-nm-wide $Al_{0.98}Mn_{0.02}$ normal metal probe (green) via a partial oxidization of the AlMn. The replica structures resulting from the shadow-mask evaporation process are also visible.(b) The measurement set-up. The current flowing through the circuit is indicated by I, and V is the voltage drop across the interferometer. L_L, L^C and L_R denote the lengths of the three arms of the weak-link.

Group Leader: Angel Rubio, University professor, UPV/EHU

09

NANOBIOSPECTROSCOPY GROUP

The “Nano-bio Spectroscopy” group focuses on the theory and modeling of electronic and structural properties in condensed matter and on developing novel theoretical tools and computational codes to investigate the electronic response of solids and nanostructures to external electromagnetic fields. Present research activities include new developments within many-body theory and TDDFT. The theoretical description of optical spectroscopy, time-resolved spectroscopies, STM/STS and XAFS is also addressed. Methodological developments include novel techniques to calculate total energies and assessment and development of exchange-correlation functionals for TDDFT calculations and improvements on transport theory within the real-time TDDFT formalism.

HIGHLIGHT

Confined linear carbon chains as a route to bulk carbine

Shi L, Rohringer P, Suenaga K, Niimi Y, Kotakoski J, Meyer JC, Peterlik H, Wanko M, Cahangirov S, Rubio A, Lapin ZJ, Novotny L, Ayala P and Pichler T.

Nature Materials 15, 634 (2016)

Researchers present a direct first proof of stable ultra-long 1D carbon chains, thus paving the way for the bulk production of carbyne

Elemental carbon appears in many different modifications, including diamond, fullerenes and graphene. Their unique structural, electronic, mechanical, transport and optical properties have a broad range of applications in physics, chemistry and materials science, including composite materials, nanoscale light emitting devices and energy harvesting materials. Within the "carbon family", only carbyne, the truly one-dimensional form of carbon, has not yet been synthesized despite having been studied for more than 50 years. Its extreme instability in ambient conditions rendered the final experimental proof of its existence elusive. An international collaboration of researchers now succeeded in developing a novel route for the bulk production of carbon chains composed of more than 6,400 carbon atoms by using thin double-walled carbon nanotubes as protective hosts for the chains. These findings are published in the journal *Nature Materials* and represent an elegant forerunner towards the final goal of carbyne's bulk production. Besides the potential applications, these findings open the possibility to answer fundamental questions about electron correlations, electron-phonon interactions and quantum phase transitions in one-dimensional materials.

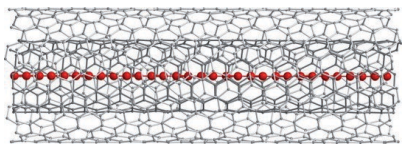


Figure: Carbon chains of increasing length have been successfully synthesized over the last 50 years.

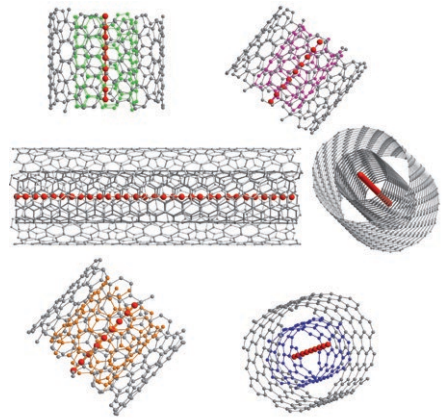


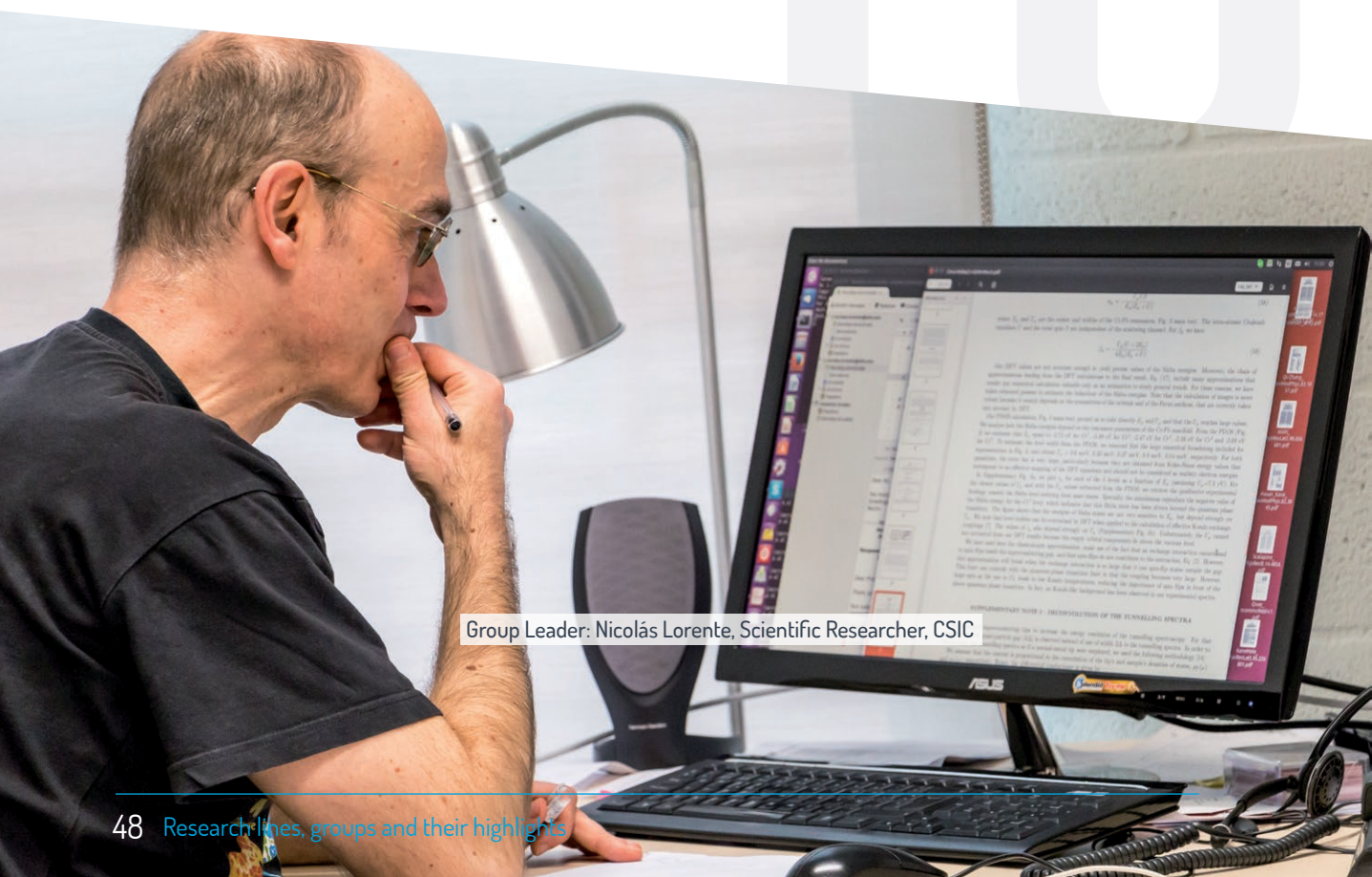
Figure: Schematic representations of confined ultra-long linear acetylenic carbon chains inside different double-walled carbon nanotubes.

So far, the record has been a chain made of around 100 carbon atoms (2003). This record has now been broken by more than a factor 50 with the first-time demonstration of micrometer length-scale chains. Researchers from the University of Vienna led by Thomas Pichler have developed a novel and simple approach to stabilize carbon chains with a record length of more than 6,400 carbon atoms. They use the confined space inside a double-walled carbon nanotube as a nanoreactor to grow ultra-long carbon chains on a bulk scale. In collaboration with the groups of Kazu Suenagas at the AIST in Japan, Lukas Novotny at the ETH Zürich and the theory group of Angel Rubio at the Max Planck Institute for the Structure and Dynamics of Matter at CFEL in Hamburg and at the CFM (UPV/EHU-CSIC) in San Sebastián, the existence of the chains has been unambiguously confirmed by using a multitude of sophisticated complementary methods.

10

QUANTUM PHENOMENA ON SURFACES GROUP

The scanning tunneling microscope (STM) probes the electronic properties of condensed-matter systems by smoothly injecting or removing electrons. Assuming that the machine does not perturb the system, the electronic structure seen by propagating an electron or a hole is exactly what the spectral function does. In other words, the STM reads the spectral function of real systems. The line of research in this group is to develop computational schemes to unveil all the richness of realistic spectral functions. The group is thus interested in electronic, vibrational and magnetic excitations. The Kondo effect is an unavoidable phenomenon of systems that present time-reversal symmetry and electron scattering. Particle pairing like in superconductors is also very exciting. Trying to understandthemany different systems and yield quantitative explanations for the several experimental data obtained in STM laboratories around the globe is also this group's goal.



Group Leader: Nicolás Lorente, Scientific Researcher, CSIC

HIGHLIGHT

Extremeley long-lived magnetic excitation in supported Fe chains

J.P. Gauyacq and N. Lorente.

Phys. Rev. B 94, 045420 (2016)

Technologically, information is stored as small magnetic moments by reversing them in complex patterns that can be read by an electronic current sensitive to the magnetic moment direction. The smallest patterns are being written using a scanning tunneling microscope that can shift a few magnetic atoms to points on a surface and build a tiny array of magnetic moments. However, at this size, quantum effects become overwhelming. This can be considered as the limit of what a future technology will be soon facing to store information. A consequence of quantum effects is the impossibility to keep a fixed magnetic pattern as is classically obtained. The lifetime of a given pattern is then very important to study how to write information that stays long enough in one of these nanomagnets. It has been found that quantum effects can actually help maintaining information in a small magnet. This is a combination of symmetry laws and interactions. In this work it is shown that recent measurements in small Fe atomic chains can be rationalized and lead to very long-lived states that are very interesting both scientifically and technologically.

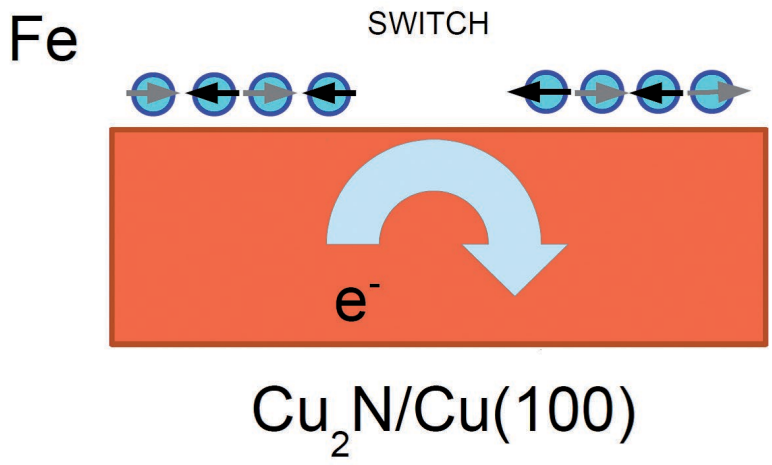


Figure: Fe chains on a copper nitrate substrate orients antiferromagnetically. In principle it is possible to write two bits by choosing one arrangement or the other as shown in the figure. In practice, quantum effects lead to an entanglement of both configurations and the destruction of a simple configuration. However, interaction with the substrate electrons can stabilize the structures and reduce the apparent switching between configurations.

Photonics

The research line on **"Photonics"** at CFM deals with the study of the interaction of radiation and matter from different and complementary approaches: (i) the theoretical research on the interaction of light with metallic and semiconductor nanostructures to confine and engineer electromagnetic fields in the nanoscale, (ii) the experimental research on the optical properties of new materials and elements that provide improved properties in a variety of lasing effects, as well as the design of novel photonic structures that provide laser confinement for bioimaging, and (iii) the experimental implementation of spectroscopy and photonic applications of nanoscale functional units, including different types of low-dimensional systems. Thus, this research line is explored by three different groups.

11

THEORY OF NANOPHOTONICS GROUP

The "Theory of Nanophotonics" group is devoted to the theoretical description of the optical properties of nanoscale structures. The interaction of light and matter is addressed by this group with techniques from condensed matter physics, as well as from quantum optics, which provide useful methodological tools to address the dynamics of excitations at the nanoscale. The understanding of light-matter interaction requires the analysis of the different time and space scales that come into play. This study is often developed in the context of different spectroscopy and microscopy configurations such as in SERS, SEIRA, STM-induced light emission, EELS, and s-SNOM. Some of the phenomena that are currently under research in this group include quantum plasmonics, acousto-plasmonics, metallic nanoantennas, field-enhanced spectroscopy and microscopy, theory of near-field microscopy, and nonlinear nanooptics, among others.

Group Leader: Javier Aizpurua, Research Professor, CSIC

HIGHLIGHT

Single-molecule optomechanics in “picocavities”

Benz F, Schmidt MK, Dreismann A, Chikkaraddy R, Zhang Y, Demetriadou A, Carnegie C, Ohadi H, de Nijs B, Esteban R, Aizpurua J and Baumberg JJ.

Science 354, 726 (2016)

For centuries, scientists believed that light could not be focused down smaller than its wavelength, just under a millionth of a meter. Researchers from the “Theory of Nanophotonics” group, in collaboration with DIPC and the University of Cambridge, have created the world’s smallest magnifying-glass which focuses light a billion times more tightly, down to the scale of single atoms. Theoretical models suggested that atoms might act as tiny lightning rods that could localize light to the atomic scale. These special cavities can enhance the coupling between photons and molecular vibrations in a Raman scattering process leading to an enhanced interaction in a tiny volume.

The experimental team in Cambridge used highly conductive gold nanoparticles to make the world’s tiniest optical cavity, so small that only a single molecule can fit within it, opening up new ways to study the interaction of light and matter. The cavity –called a ‘pico-cavity’ by the researchers – consists of a bump in a gold nanostructure the size of a single atom, and confines light to less than a billionth of a meter (see figure A).

In the same way as a hand plucks the strings of a guitar, the energy of light can activate the vibrations of a particular bond in a molecule. This phenomenon is called optomechanical interaction, and in this work, the researchers have achieved that light localized at the picocavity can “pluck” the vibrations of a nearby molecule. This can be understood as the tiniest guitar in the world, a “molecular guitar” activated by light. This molecular optomechanical interaction can be used to switch optical signals, i.e. to “play” particular notes in the molecular “guitar”: certain light plays some notes, and others are not capable to activate them, thus allowing for switching the molecular signal with light at the tiniest scale, the atomic scale.

11

THEORY OF NANOPHOTONICS GROUP

Building nanostructures with single atom control is extremely challenging and it required cooling the samples to -260°C in order to freeze the scurrying gold atoms. The researchers shone laser light on the sample to build the pico-cavities, allowing them to watch single atom movement in real time. Single gold atoms behave just like tiny metallic basketballs that trap light thanks to the behavior of their electrons roaming around. They used this to blend light together with mechanical springs based on single vibrating bonds, which allows molecular motion to be used for tiny switches. The optomechanical interaction in the tiniest picocavities was reported by monitoring the anti-Stokes signal of a single molecule. The quadratic evolution of the anti-Stokes signal is a clear fingerprint of the effect of vibrational pumping of the molecule's vibration induced by the picocavity (see Figure B).

The control of molecular vibrations in nanoscale environments has the potential to open a whole new field of light-catalyzed chemical reactions, allowing complex molecules to be built from smaller components, as well as make new opto-mechanical devices.

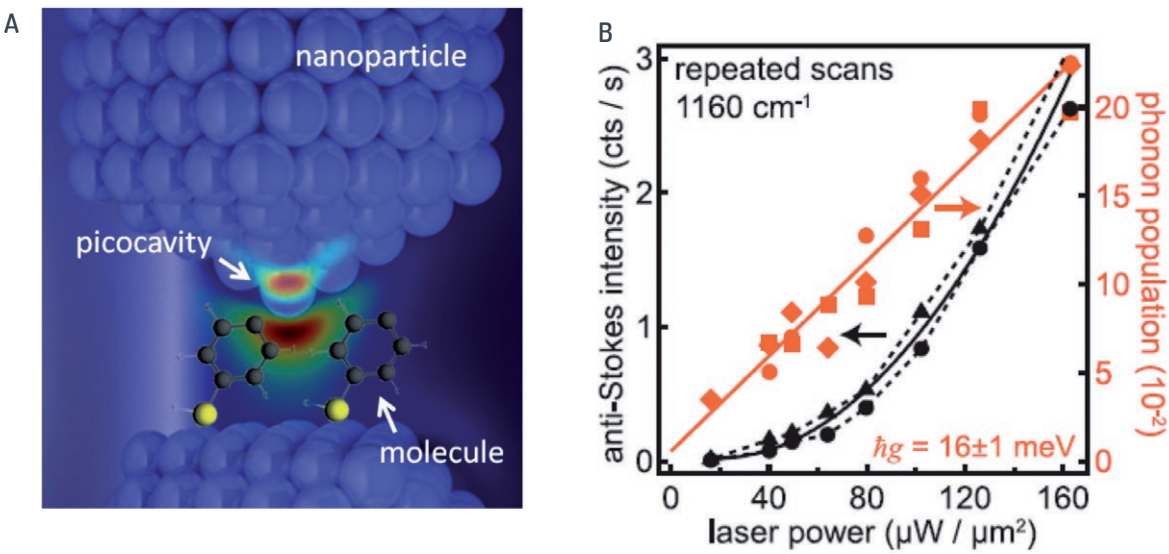


Figure: (A) Artistic composition that shows a molecule in the proximity of a "picocavity" where the field of a plasmonic nanoparticle is focused down to the atomic scale, producing effects of molecular optomechanical coupling. The blue spheres represent atoms of a metallic lattice in a nanoparticle and the local field distribution is represented with red and green colors depending on the intensity of the field, according to ab-inition calculations of the atomic-scale localization of the optical response. (B) Evolution of the anti-Stokes intensity (black line and symbols) of the 1160cm-1 vibration of a biphenyl-4-thiol molecule in a monolayer located in a plasmonic picocavity, as a function of the incident laser power. A quadratic dependence of the aS signal is observed. The corresponding phonon population evolution is depicted in orange.

12

NANOMATERIALS AND SPECTROSCOPY GROUP

The “Nanomaterials and Spectroscopy” group is focused on spectroscopy and photonic applications of nano-scale functional units, including semiconductor quantum dots and quantum wires, metal nanoparticles and nanoantennas, and organic/inorganic nano-hybrid systems. Further research activity in the group includes the study of optical properties in semiconductor nanocrystals (quantum dots), nano-hybrid materials, heterostuctures (quantum wires), metal nanoparticles, nanoantenas and organic functional materials (J-aggregates), as well as novel experimental approaches to control, manipulate and probe with light on nanoscale.

Group leader: Yury Rakovich, Ikerbasque Research Professor, UPV/EHU

HIGHLIGHT

Rabi Splitting in Photoluminescence Spectra of Hybrid System of Gold Nanorods and J-aggregates

Dzmitry Melnikau, Ruben Esteban, Diana Savateeva, Ana Sánchez-Iglesias, Marek Grzelczak, Mikolaj Schmidt, Luis Liz-Marzan, Javier Aizpurua and Yury Rakovich.

Journal of Physical Chemistry Letters, 7, 354 (2016)

One of the main objectives of nanophotonics research is the control of the light-matter interaction on the nanoscale. The coupling between plasmonic and excitonic resonances (plexitonic coupling) is of great interest for fundamental studies and for many practical applications. The interaction between plasmons and excitons strongly affects energy and electron-transfer pathways and, as a result, absorption and emission properties. For many applications the so-called strong coupling regime is especially attractive, which is produced when the rate of coherent energy exchange between the excitonic and plasmonic systems exceeds the rate of the losses in the system. In this regime the two new hybrid states are generated, both having features of light and matter. These new states are separated by an energy called Rabi splitting.

While observation of Rabi splitting in extinction or transmission spectra of plexitonic structures that combine metal nanoparticles and molecular systems has been reported in a number of publications, photoluminescence properties of a plexitonic hybrid system in strong coupling regime remained more elusive to experimental investigation.

In this work the interactions between localized plasmons in gold nanorods and excitons in supramolecular J-aggregates were experimentally and theoretically investigated.

The evolution of the two extinction and emission peaks separated by Rabi energy was followed as the plasmon energy was gradually detuned from the excitonic resonance. By this way, clear anticrossing behavior of the hybridized modes was demonstrated not only in the extinction but (for the first time) also in the photoluminescence spectra of this system. Both the extinction and photoluminescence results were found to be in good agreement with the theoretical predictions obtained for the model that assumes two interacting modes with a significant Rabi splitting of ~200 meV. It turned out that the evolution of the photoluminescence line shape with increasing detuning depends on the illumination wavelength. This effect was attributed to an incoherent excitation given by decay processes in either the metallic rods or the J-aggregates.

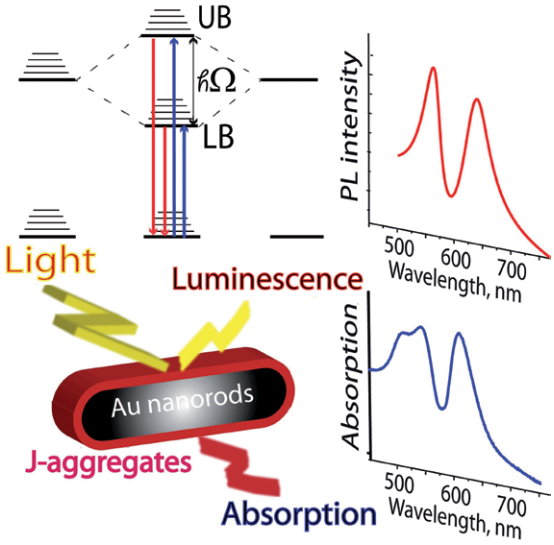


Figure: Rabi splitting in absorption (right, bottom) and photoluminescence (right, top) spectra of hybrid system of gold nanorods and J-aggregates (left, bottom). Schematic on the left (top) shows formation of lower (LB) and upper (UB) bands as a result of exciton-plasmon interaction.

Group Leader: Rolindes Balda, University Professor, UPV/EHU

13 LASER PHYSICS AND PHOTONIC MATERIALS GROUP

The "Laser Physics and Photonic Materials" group is located in the Department of Applied Physics of the School of Engineering of the University of the Basque Country (UPV/EHU) in Bilbao, and devotes most of its research efforts to the optoelectronic properties of new materials and structures for solid state lasing and photonic crystal properties. Its activity also covers the development of a complete set of high resolution techniques, the development of new low-energy phonons, rare earth-doped dielectric materials for energy converters and/or solid state laser cooling applications, and the probing, characterizing and modeling transport and/or confinement of ultrafast ultra-intense laser light in inhomogeneous (nano-micro) dielectric materials doped with optically active centers for nanosensors, displays, and bioimaging applications.

HIGHLIGHT

Influence of Upconversion Processes in the Optically-Induced Inhomogeneous Thermal Behavior of Erbium-Doped Lanthanum Oxysulfide Powders

Balda R, Hakmeh N, Barredo-Zuriarrain M, Merdrignac-Conanec O, Garcia-Revilla S, Arriandiaga MA and Fernandez J.

Materials 9, 353 (2016)

Lasers are commonly known as sources of heat used to burn or cut through tissue and other materials, but when shone on certain solids doped with rare-earth ions, a laser can cool down the material. The basic principle that anti-Stokes fluorescence might be used to cool a material was first postulated by P. Pringsheim in 1929. Twenty years later A. Kastler suggested that rare-earth-doped crystals might provide a way to obtain solid-state cooling by anti-Stokes emission (CASE).

13

LASER PHYSICS AND PHOTONIC MATERIALS GROUP

An anti-Stokes emission occurs when a material emits more energy than it absorbs. The key is to shine photons onto the material that fall short of the energy needed to excite the rare earth ions to a higher energy level. The material uses the energy from thermal vibrations to make up the difference. Whenever a quantum of these thermal vibrations is absorbed, an ion is excited to a higher energy state and then fluoresces, carrying energy out of the system and cooling the material.

The group is currently investigating Er^{3+}-doped Lanthanum oxysulphide crystal powders as a promising candidate for all-optical cooling. This material, with maximum phonon energy of about 400 cm^{-1} exhibits an efficient infrared to-visible upconversion under excitation in the 800–870 nm spectral region. The team has analyzed the thermal response of Er-doped lanthanum oxysulphide powders by pumping with a tunable femtosecond laser working at 80 MHz.

Figure (a) shows a typical video frame of the sample after irradiation. As can be seen, the temperature distribution is rather inhomogeneous showing a sharp distribution of hot spots. Figure (b) displays the average temperature as a function of time measured in the three shown zones.

Initially, the temperature of the sample rises in all the zones from room temperature (~ 24 °C) till it reaches a stationary regime when the thermal load deposited on the material is compensated by the fluorescent losses. As can be seen, in the hot zone, E2, the temperature falls by 2 °C in forty minutes whereas in the wider one, E1, the average temperature drops about 0.5 °C. These results are in good agreement with the expected random propagation of radiation in a region with a randomly distributed dielectric constant.

Finally, it is worthy to point out that the average temperature of the sample may cool after the initial transient heating due to the infrared to visible upconversion processes that can offset the heat load deposited in the doped powder.

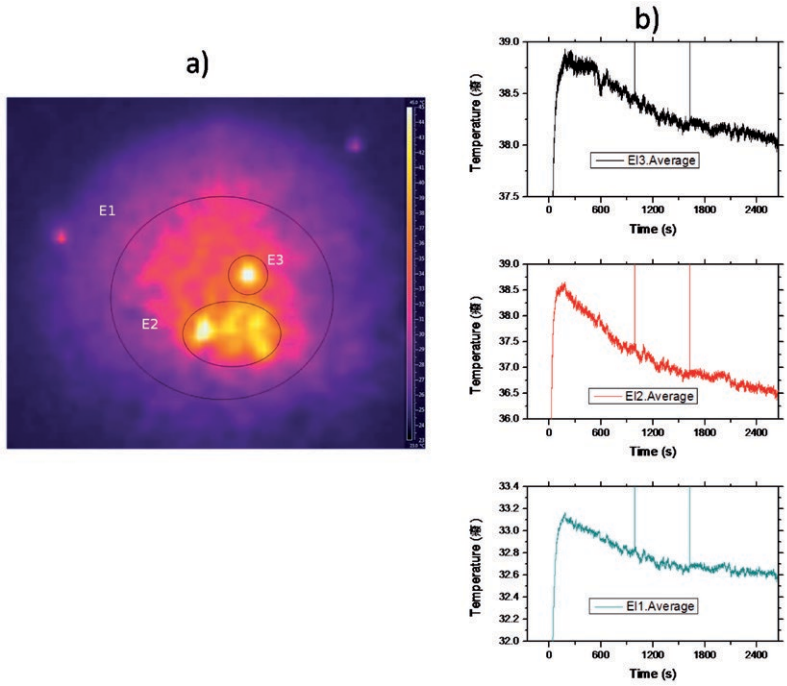


Figure: (a) Camera video frame showing discrete thermal zones after pumping with 300 mW at 842 nm in a 2 mol% Er^{3+}-doped La_2O_2S powder sample. (b) Average temperature as a function of time measured in the three shown zones in (a).

Polymers and Soft Matter

14 POLYMERS AND SOFT MATTER GROUP

This research line is also categorized as a research group. The Group of “Polymers & Soft Matter”, led by Professor J. Colmenero, covers a research activity on “Polymers and non-Crystalline Materials”.

Taking inspirations from classical polymer science, soft matter science and the physics of condensed matter, the group has developed over the last years a pioneering methodology to investigate structure and dynamics of polymer and glass-forming systems in general at different length and time scales. This methodology is based on the combination of relaxation techniques, neutron and X-ray scattering, microscopy techniques and molecular dynamics simulations. The organization of the group is in fact driven by this methodology and the staff of the group is composed of experts in different techniques/methods, all of them being involved in the scientific objectives defined at any time.

Recently, the group has strengthened its capabilities in chemical synthesis oriented to polymers. These capabilities are of utmost importance to break into the general arena of soft matter sciences.

Group Leader: Juan Colmenero, University Professor, UPV/EHU

POLYMERS AND SOFT MATTER GROUP

HIGHLIGHT

Dielectric Susceptibility of Liquid Water: Microscopic Insights from Coherent and Incoherent neutron scattering

Arbe A., Malo de Molina P, Alvarez F., Frick B. and Colmenero J.

Physical Review Letters 117 (2016) 185501

Paper selected as Editors' Suggestion and Featured in *Physics*

Water is an extremely complex liquid, made of networks of H_2O molecules linked by hydrogen bonds that continuously form and break. Most of our knowledge of the liquid comes from spectroscopic studies—dielectric relaxation, Raman scattering, infrared absorption, and x-ray or neutron scattering—which use radiation or particles to probe different aspects of atomic and molecular motions. The combined information derived from all these techniques may provide a coherent picture of the liquid's dynamics, shedding light on important questions about the nature of water. How do molecular phenomena, such as vibrations, rotations, diffusion, and the making and breaking of hydrogen bonds determine the macroscopic properties of water, including its large dielectric constant? What are the mechanisms by which the liquid relaxes when energy is deposited into it? What is the distance over which molecules of water can "feel" each other —the so-called correlation length?

The authors of this work combine results from measurements of dielectric relaxation and neutron scattering to deliver a detailed and unified picture of water dynamics at room temperature. Through dielectric relaxation experiments, the collective relaxation of electrical dipoles that determines the macroscopic dielectric response of water is characterized. Thanks to the atomic scale sensitivity of neutron scattering measurements, the authors were then able to establish a relationship between molecular dynamics and the dielectric behavior of the liquid.

The main feature of dielectric relaxation measurements is a peak in e"(n) centered at 20 GHz (see Figure). This is the well-known Debye peak, indicating that the collective relaxation of the macroscopic dipole moment occurs on a time scale of 8.3 ps. By means of neutron scattering, the authors of this paper have shown that the same peak is seen when the (incoherent) neutron scattering susceptibility is measured at a momentum transfer of $Q = 7\ nm^{-1}$. The Q dependence of the peak position demonstrates that dipolar relaxation is linked to molecular diffusion and gives the length scale of collective dipolar relaxation. The researchers deduce that the 8.3-ps dynamics is due to the movement of atoms along relatively large distances (0.34 nm), which are comparable to or slightly larger than intermolecular distances.

As in the case of dielectric relaxation, the authors' neutron scattering experiments also reveal two smaller peaks in the THz domain, a high-frequency range hardly accessible by dielectric relaxation. Because their position doesn't change with Q, the peaks correspond to localized motions. The peak at the highest frequency (around 2 THz) is associated with bending of chains of three oxygen molecules connected by hydrogen bonds (O—O—O). The other one, at intermediate frequencies (around 0.15 THz), is a novel finding of this work. This peak is related to local processes—motions of hydrogen atoms that take place when intermolecular bonds break and reform on picosecond time scales.

These results confirm the presence of two relaxational processes in liquid water, which are related to

the diffusion of molecules and local movements associated with the making and breaking of hydrogen bonds, respectively.

This picture is similar to that observed in polymers, which involves two main types of relaxation —called a (diffusion-like) and b (localized motions)— taking place on different spatial and temporal scales. This description also opens a new way of approaching dynamics of water under different conditions (supercooled, confined, biological water, etc.) and that of other H-bonded liquids.

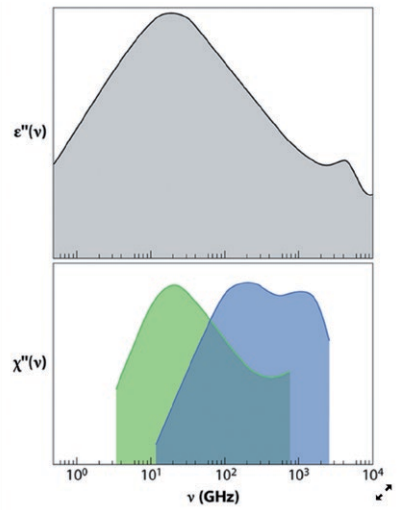


Figure: (Top) Dielectric relaxation measurements of water at 298 K reveal a 20-GHz peak in the imaginary part of the dielectric constant and hints of further peaks at higher frequencies. (Bottom) Neutron scattering data at Q= 7 nm-1(green) indicate the 20-GHz peak is due to molecular diffusion. Data at Q= 20 nm-1 (blue) reveal two high-frequency peaks at 0.15 and 2 THz and suggest they originate from local motions of hydrogen and oxygen atoms.

HIGHLIGHT

Concentrated solutions of single chain nanoparticles: a simple model for intrinsically disordered proteins under crowding conditions

Moreno AJ, Lo Verso F, Arbe A, Pomposo JA and Colmenero J.

Journal of Physical Chemistry Letters 7, 838 (2016)

Single-chain nanoparticles (SCNPs) are an emergent class of soft nano-objects with promising applications in e.g., nanomedicine, biosensing, bioimaging, or catalysis. They are synthesized through intramolecular cross-linking of polymer precursors. In this work, the research team performed a detailed simulation analysis of the conformations of SCNPs, revealing that they share basic ingredients with intrinsically disordered proteins (IDPs), as topological polydispersity, compact domains and sparse regions.

IDPs are highly abundant in eukaryotes. Their biological function is founded on their internal dynamics and flexibility, enabling them to respond quickly to environmental changes and to bind with different cellular targets. As a direct consequence of their malleability,

the structural, dynamic and associative properties of IDPs can be affected by macromolecular crowding in vivo, substantially differing from the observations in vitro at highly dilute conditions.

The research team exploited the structural analogies between SCNPs and IDPs and investigated the conformational properties of SCNPs in concentrated solutions. SCNPs provide a model system that shares universal structural features with IDPs and is free of specific interactions, allowing to investigate separately the purely steric excluded-volume contributions to crowding. For this purpose, large-scale simulations of a generic bead-spring model for solutions of SCNPs and small-angle neutron scattering (SANS) experiments on real systems were combined, covering the whole concentration range from infinite dilution to melt density. The role of the internal degree of disorder of the SCNP on its collapse behavior under macromolecular crowding was analyzed.

It was found that crowding leads to collapsed conformations of SCNPs resembling those of the crumpled globular class. This behavior was already found at volume fractions (about 30 %) that are characteristic of crowding in living cells.

The results in SCNPs propose a universal scenario for IDPs: steric crowding in cell environments lead IDPs to adopt crumpled globular conformations. The usual transition from self-avoiding to random coil (Gaussian) conformations found in linear macromolecules is only a particular case, taking place in the limit of fully disordered IDPs.

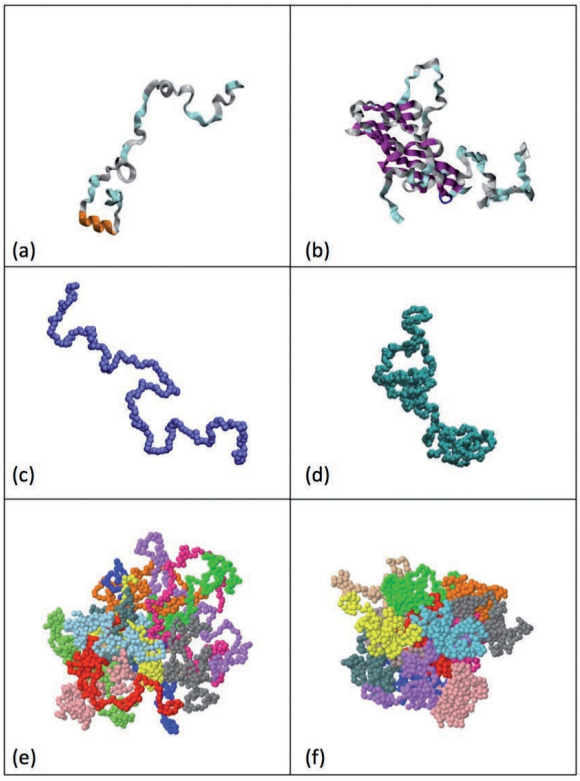


Figure: (a): IDP in the limit of full disorder. (b): IDP with a compact domain. (c): Polymer chain. (d): SCNP. (e): Concentrated solution of polymer chains, showing Gaussian confornations. (f): Concentrated solution of SCNPs, showing crumpled globular conformations.

SELECTED REVIEW

Confined Water as Model of Supercooled Water

Cerveny S, Mallamace F, Swenson J, Vogel M and Xu LM.

Chemical Reviews 116, 7608 (2016)

Water is a key compound for the existence of life since it is involved in almost all the chemical, geological and biological processes that occur on our planet. Although water is the most common liquid, it is also the most unusual with many atypical properties. These anomalies become more pronounced in the no man's land region (150 - 230 K) where bulk water immediately crystallizes into ice. One way to avoid crystallization of water is to restrict the size of water domains by different types of geometrical confinements. In this way, it is possible to experimentally access this temperature region avoiding crystallization. These confinements are also observed in geological systems and in the new nano-technological materials. Moreover, many biological processes take place in very small aqueous environments where water can be considered to be confined in small cavities. Since the presence of confined water is essential for life, the importance of understanding its dynamic and structural properties is extremely relevant.

For this reason a group of scientists, with different and controversial opinions on the subject of the dynamical behavior of confined water at low temperatures, gathered to give a new vision on this subject. Consequently, this review is not a typical compilation of data previously measured; instead the group of experts provided an integrative approach of this problem. To achieve this challenge, three experimental techniques have been used: dielectric spectroscopy, nuclear magnetic resonance and quasi-elastic neutron scattering. We have proposed three different scenarios for the dynamics of confined water (see Figure). However, from these studies it is also clear that the interpretations of the experimental data are far from evident. Therefore, three main interpretations are presented to explain the experimental data, with a discussion of their advantages and disadvantages. Unfortunately, none of the proposed scenarios is able to predict all the observations for supercooled and glassy bulk water, indicating that either the structural and dynamical alterations of confined water are too severe to make predictions for bulk water or the differences in how the studied water has been prepared (applied cooling rate, resulting density of the water, etc.) are too large for direct and quantitative comparisons.

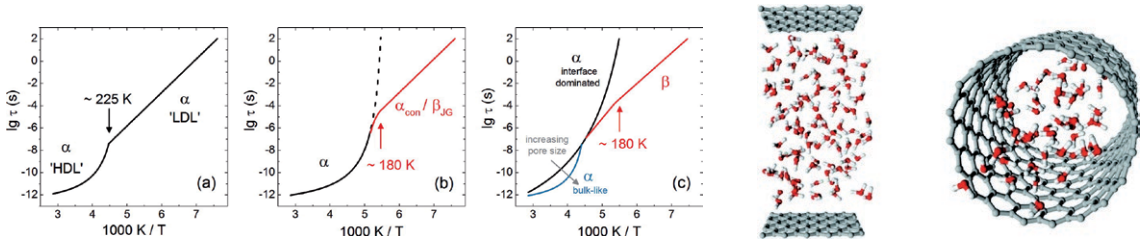


Figure: Schematic diagram at ambient pressure of different scenarios for the dynamical behavior of supercooled confined water. α_{conf} indicate confined α-relaxation, and β_{JG} means Johari-Goldstein β-relaxation. On the right, some confinements used are shown.

FACILITIES

FACILITIES

CFM routinely uses several services and techniques to internally develop the activity within the research lines as well as to launch competitive projects funded by different agencies. All the infrastructure of CFM laboratories is readily available to be used for development of external research projects through our External Services Offer. This is a fast, reliable, scalable and economically competitive way of obtaining valuable characterization data using any of our state-of-the art techniques. Additionally, our researchers can provide consultancy services for interpretation of this information and advice on how to use it efficiently. All requests are treated in full confidentiality.

COMPUTING FACILITIES

Two High Performance Computing clusters adding up a total of 2088 computing cores and 6TB of memory, 72TB of shared, replicated, storage space, as well as a variety of workstations for small calculations and software development.

ULTRA-LOW TEMPERATURE SCANNING TUNNELING MICROSCOPY LAB

A combined AFM/STM instrument capable of scanning atomic forces and tunneling current simultaneously at 1 K.

HIGH RESOLUTION ANGLE RESOLVED PHOTOEMISSION LAB

A combined ARPES/STM system with a double prep-chamber, which permits separate and joint ARPES/STM experiments. The ARPES chamber is an ultra-high resolution (0.1 degree, 5 meV) system, able of measuring solid samples down to 20 K.

SURFACE CHEMISTRY AND MAGNETISM LAB

Two separate STM/X Ray Photoemission (XPS) and STM/Magneto Optic Kerr Effect (MOKE) chambers for surface chemistry and surface magnetism experiments, respectively.

FACILITIES

NANOPHOTONICS LAB

Scanning confocal time-resolved photoluminescence setup (MicroTime200, PicoQuant) providing single molecule sensitivity and high temporal resolution. Range of application includes Fluorescence Lifetime Imaging (FLIM), Fluorescence Correlation Spectroscopy (FCS), Forster Resonance Energy Transfer (FRET), Fluorescence Lifetime Measurements, Fluorescence Anisotropy and Intensity Time Traces.

SPECTROSCOPY TECHNIQUES

Spectroscopic equipment (Cary50, Varian) for measurement of energy transfer and conversion.

LASER SPECTROSCOPY LAB

Continuous and time-resolved (with nano-pico excitation laser sources) spectroscopies with high spectral resolution in the UV-VIS-IR domains together with low temperature facilities (2K). Home made photoacoustic spectrometer.

ULTRAFAST SPECTROSCOPY LAB

Tunable femtosecond sources (with regenerative amplification) in the IR domain with shigh speed detectors in the picosecond domain (Streak camera). Multiphoton microscope with time-resolved spectroscopic facilities.

MATERIAL SYNTHESIS LAB

Crystal growth facilities by using home made Bridgman and Czochralski fournaces.

DIELECTRIC SPECTROSCOPY LAB

Different frequency and time-domain spectrometers covering more than 16th orders of magnitude in frequency/time.

MOLECULAR SPECTROSCOPY TECHNIQUES

Infrared Spectrometer FT-IR, Terahertz Spectrometer.

MICROSCOPY LAB

Atomic Force Microscope (AFM), Optical/Confocal Microscope, Desktop Scanning Electron Microscope.

X-RAY LAB

Small Angle X-Ray Scattering (SAXS) technique: Rigaku PSAXS-L, Wide Angle X-Ray Scattering (WAXS) with the same instrument.

THERMAL ANALYSIS TECHNIQUES

Differential Scanning Calorimetry (DSC), Pressure-Volume-Temperature (PVT), Thermogravimetric Analysis (TGA), Dilatometry (DIL).

MECHANICAL CHARACTERIZATION TECHNIQUES

Rheometry with simultaneous electric impedance analysis, Miniature Material Tester.

CHEMISTRY LAB

Different techniques oriented to Polymer Synthesis and Click-Chemistry.

RESEARCH OUTPUT

RESEARCH OUTPUT

RESEARCH OUTPUT

Articles

ISI publications in 2016: **211***

Publications Q1 in 2016: **178** (84,3%)

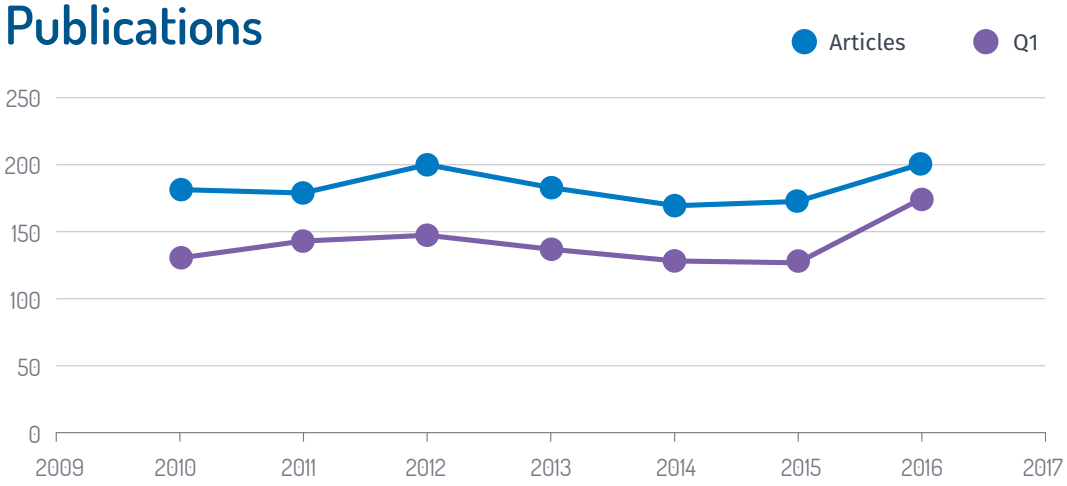
h-index: **99**

Average Impact factor of the Center in 2016: **6,497**

ISI Web of Science Citations as of April 2017: **9.473** (Total number since 2000: **65.756**)

Among all the articles published at CFM-MPC, **80.5 %** of the articles (170 out of 211) were published in the framework of international collaborations, showing the international dimension and positioning of the Center in the field of Materials Science.

Publications



** Source Web Of Science Core Collection-ResearchersID F-4867-2012*

	Articles	Q1
2010	181	134
2011	179	144
2012	198	149
2013	184	139
2014	171	131
2015	173	129
2016	211	178

Total number of publications in and above Physical Review Letters: 60

Journal	Number of articles	Impact factor
Nature Materials	1	38,891
Chemical Reviews	1	37,369
Nature Nanotechnology	2	35,267
Science	1	34,661
Nature chemistry	1	27,893
Progress in Polymer Science	1	27,184
Advanced Materials	1	18,960
Nano Letters	12	13,779
Light-Science & Applications	1	13,600
ACS Nano	6	13,334
Journal of the American Chemical Society	4	13,038
Angewandte Chemie-International	1	11,709
Advanced Functional Materials	1	11,382
Nature Communications	6	11,329
Chemistry Of Materials	1	9,407
Nano Research	1	8,893
Phase Transitions	1	8,858
Journal Of Physical Chemistry Letters	6	8,539
Small	2	8,315
Nanoscale	3	7,760
Physical Review Letters	7	7,645

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Scholl JA, Garcia-Etxarri A, Aguirregabiria G, Esteban R, Narayan TC, Koh AL, Aizpurua J, Dionne JA.
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8 Plasmonic Response of Metallic Nanojunctions Driven by Single Atom Motion: Quantum Transport Revealed in Optics
Marchesin F, Koval P, Barbry M, Aizpurua J, Sanchez-Portal D.
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9 Anomalous Spectral Shift of Near- and Far-Field Plasmonic Resonances in Nanogaps
Lombardi A, Demetriadou A, Weller L, Andrae P, Benz F, Chikkaraddy R, Aizpurua J, Baumberg JJ.
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10 Multiphase Biomineralization: Enigmatic Invasive Siliceous Diatoms Produce Crystalline Calcite
Ehrlich H, Motylenko M, Sundareshwar PV, Ereskovsky A, Zglobicka I, Noga T, Plocinski T, Tsurkan MV, Wyroba E, Suski S, Bilski H, Wysokowski M, Stocker H, Makarova A, Vyalikh D, Walter J, Molodtsov SL, Bazhenov VV, Petrenko I, Langer E, Richter A, Niederschlag E, Pisarek M, Springer A, Gelinsky M, Rafaja D, Witkowski A, Meyer DC, Jesionowski T, Kurzydlowski KJ.
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13 Growth of Co Nanomagnet Arrays with Enhanced Magnetic Anisotropy
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21 The role of PLLA-g-montmorillonite nanohybrids in the acceleration of the crystallization rate of a commercial PLA
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22 Tailored pump-probe transient spectroscopy with time-dependent density-functional theory: controlling absorption spectra
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24 Andreev spectrum of a Josephson junction with spin-split superconductors
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30 **Electron-phonon relaxation and excited electron distribution in gallium nitride**
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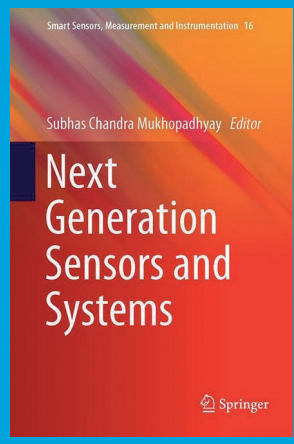

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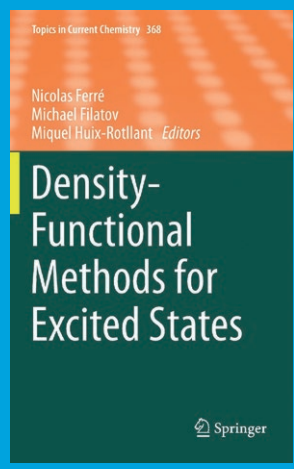
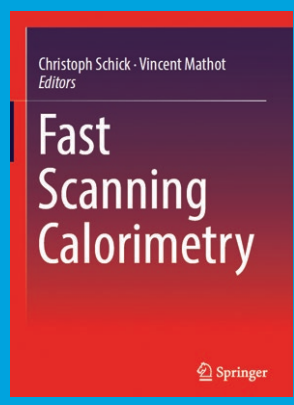
  TOPICS IN CURRENT CHEMISTRY
  Density-Functional Methods for Excited States 368, 219 (2016)



- **Cooling Rate Dependent Glass Transition in Thin Polymer Films and in Bulk**
  Cangialosi D, Alegría A, Colmenero J.
  Fast Scanning Calorimetry, 403 (2016)




MECHANICS
Solid State Physics
TRAINING

TRAINING

TRAINING

The Materials Physics Center (CFM-MPC) is a joint institute embedded in the academic activity of the University of the Basque Country (UPV/EHU) and thus it shares the mission of the University regarding higher education, in particular at post-graduate level. CFM-MPC is one of the very few centers of the Basque Country in which a balanced body of University teachers/scientific researchers (CSIC and Ikerbasque researchers) coexist and interact on a regular basis, transferring many of the values of the collaboration between university faculty and research center to the classroom. The standard higher education available to a student at CFM is associated to two degrees awarded by the corresponding departments at UPV/EHU:

Master in Nanoscience

This is an official master program of UPV/EHU (held at CFM headquarters) and co-organized by CFM-MPC itself. The goal of the Master in Nanoscience is to provide the student with the basic concepts and the most common working tools in the field of Nanoscience, including the use and interpretation of the results of experimental techniques that are specific to Nanotechnology research laboratories, several topics related to nanomaterials and their applications, and a general knowledge on the research activity at the international level in the field of Nanoscience. More specifically, a focus on electronic, magnetic, dielectric and optical properties of nanoscale materials is developed during the course.

In addition, during their Master's thesis work, students choose to develop the skills either in fields directly linked with applied and technology-oriented research work in Technological Centers, or in the basic/oriented research that is carried out in academic research groups. The students will be also able to start developing the research work that may allow them to access the PhD program. The list of master theses successfully defended at CFM in 2016 follows:

Master Theses defended in 2016

- **Infrared spectroscopy of antennas on hexagonal boron nitride**
  Student: Biolek Vladimír
  Supervisors: R. Hillenbrand and A. Nikitin

- **Enzyme-Mimetic Synthesis of PEDOT Conducting Polymer using Iron-Containing Metallo-Folded Single-Chain Polymer Nanoparticles**
  Student: Julen de la Cuesta Leone
  Supervisor: J.A. Pomposo

- **Quantum description of superradiant emission from single emitters coupled with plasmonic nanoparticles in asymmetric configurations**
  Student: Gabriela Olivíková
  Supervisors: R. Esteban Llorente and J. Aizpurua Iriazabal

- **Optical properties of semiconductor quantum dots: from ensembles to single dot studies**
  Student: Herman Borovkov
  Supervisor: Y. Rakovich

- **Anharmonic renormalization of flexural acoustic modes in graphene**
  Student: Unai Aseginolaza Agirretxe
  Supervisors: A. Bergara and I. Errea

PhD program on "Physics of Nanostructures and Advanced Materials"

This is a Ph.D. program of the University of the Basque Country (UPV/EHU) which has been recognized by the Spanish Ministry of Education as a highly qualified Ph.D. program (*Mención hacia la excelencia* MEE2011-0591). After completing a master program (the Master's in Nanoscience program, or other similar degrees), the PhD student joins one of the research groups at the Center and is trained to develop his/her own research work. The PhD Committee of Graduate Studies looks after the PhD student's training on an individual basis. The list of PhD thesis projects successfully defended at CFM in 2016 follows:

PhD Theses

- **Size-dependent electronic properties of metal nanoparticles**
  Student: Marina Quijada Van der Berghe
  Supervisor: R. Díez
  14/01/2016

- **Classical and quantum approachis to the interaction of light and matter at the nanoscale**
  Student: Mikolaj Kajetan Schmidt
  Supervisor: J. Aizpurua
  15/01/2016

- **Analysis and control or transient spectra using time-dependent density fuctional theory**
  Student: Jessica Walkenhorst
  Supervisors: A. Rubio and A. Castro
  29/01/2016

- **Interaction of ions, electrons, and laser pulses with surfaces**
  Student: Iñigo Aldazabal Mensa
  Supervisors: A. Arnau and V. H. Ponce
  29/01/2016

- **Structure and Dynamics of Unentangled Polydimethylsiloxane: Molecular Dynamics Simulations validated bay Scattering Experiments**
  Student: Maria Luisa Barceló Hernandez-Gil
  Supervisors: J. Colmenero de León and F. Álvarez
  05/02/2016

- **Electron dynamics in the interaction of atomic particles with spherical metal clusters**
  Student: Natalia Koval
  Supervisors: R. Muiño and D. Sánchez-Portal
  22/04/2016

- **Modeling and analysis of thermoelectric energy convesion efficiency in nanoestructures**
  Student: Yang Kaike
  Supervisors: R. D´Acosta and A. Rubio
  22/06/2016

- **Análisis estructural de aleaciones ligeras de Boro y As2Te3 a altas presiones**
  Student: Ainhoa Suárez Alcubilla
  Supervisors: A. Bergara and I. García de Gurtubay
  14/10/2016

- **Theoretical study on the photoswitching mechanism of negative reversibly photoswitchable fluorescent proteins**
  Student: Bruno Torcal
  Supervisors: M. Wanko and A. Rubio
  26/10/2016

- **Phonon and electron excitations in abstraction processes from metallic surfaces**
  Student: Oihana Galparsoro
  Supervisors: Maite Alducin and Pascal Larrégaray
  14/12/2016

- **Elementary reactive processes of nitrogen and hydrogen on metal surfaces: A theoretical study**
  Student: Mohamed Ahmed Nosir
  Supervisor: R. Diez
  16/12/2016

- **Dielectric relaxation and structure of complex materials: supramolecular ensembles and hybrid adhesives**
  Student: Gerardo Martinez
  Supervisor: A. Alegria
  20/12/2016

Undergraduate Courses

In addition to the Master's and PhD programs, the staff at CFM also participates in a variety of undergraduate courses in 4 Faculties and University Schools of the University of the Basque Country (UPV/EHU). In total, more than 1400 teaching hours spread over 6 undergraduate degrees and 3 Master degrees at UPV/EHU are delivered by CFM staff.

PhD students seminars

Since 2013, a regular series of seminars delivered by PhD students is organized at CFM. This activity continued during 2016. Approximately every two weeks, from September to June, two PhD students present updated results of their thesis work to the full CFM research community. Two other PhD students assume the role of opponents and are in charge of asking questions and discussing the presented results. The most important goal of this activity is to train PhD students in the necessary habits of science communication and research discussions. Furthermore, it helps to improve the internal communication about the research activity going on in the Center.

- **Ivor Loncaric**
  "Dynamics of CO scattering and adsorption on Ru(0001): microscopical elucidation of the results of molecular beam experiments"

- **Oihana Galparsoro**
  "Phonon and electron excitations in abstraction processes from metallic surfaces"

- **Anton Brion**
  "CO adsorption on vicinal Pt(111) surfaces: role of strain unveiled by core-level spectroscopy"

- **Gerardo Martinez**
  "Dielectric relaxation analysis of hybrid Acrilyc-Polyurethane gels"

- **Marc Barbry**
  "New Developments in our Linear-Response TDDFT code"

- **Nestor Merino**
  "Structure-property relation in atomically precise graphene nanoribbons on Au(111)"

- **Moritz Mueller**
  "Influence of structural fluctioations on the lifetimes of adsorbate states at hybrid organic-semiconductor interfaces"

- **Iker Gallardo**
  "Properties of metallic atoms in different chemical environments"

- **Mattin Urbieta**
  "Spectroscopy of metallic icosahedral nanoparticles"

- **Robert Biele**
  "Time-Dependent Thermal Transport Theory and Applications"

- **Federico Marchesin**
  "Plasmonic Response of Metallic Nanojunctions Driven by Single Atom Motion"

- **Bernhard Krez**
  "Origins of contact resistance in graphene-metal edge-contacts"

- **Mohamed Nosir**
  "Theoretical Study of Nitrogen Interactions on Fe(111) Surface"

- **Kaike Yang**
  "Density functional theory for the calculation of thermoelectric power in the Coulomb blockade regime"

Internship

Undergraduate students are also offered the possibility to be trained in-situ at CFM-MPC, with the opportunity to interact with top quality research groups in summer internships.

MPC provided two summer internships to undergraduate students during 2016:

- **Alberto Hijano Mendizabal** (with Professor E. Ortega)

- **Beñat Jimenez Urbieta** (with Dr. I. Aldazabal)

WORKSHOPS
CONFERENC

WORKSHOPS AND CONFERENCES

WORKSHOPS AND CONFERENCES

CFM scientists have organized or co-organized several international workshops and conferences during 2016. Many of these meetings have been held in close cooperation with the foundation **Donostia International Physics Center (DIPC)**, which is an example of the excellent results brought by the synergistic collaboration between both institutions.

The list of workshops organized or coorganized by CFM researchers during 2016 follows:

- **Modelado multifísico - modelos basados en ecuaciones y optimización**
  April 13, 2016
  Coorganized by Addlink, CSIC and Iñigo Aldazabal (CSIC)
  Donostia-San Sebastián (Centro de Física de Materiales, CFM)

- **Energy Materials Nanotechnology: Meeting on Droplets**
  May 9-13, 2016
  Coorganizer at CFM: Yury Rakovich (UPV/EHU)
  Donostia- San Sebastián

- **Towards Reality in Modelling of Molecular Electronics**
  June 13-17, 2016
  Coorganizers at CFM: Daniel Sánchez-Portal (CSIC) and Pedro Brandimarte (CSIC)
  Donostia-San Sebastián

- **iPolymorphs. Novel Routes to Inorganic Polymorphs**
  June 22-24, 2016
  Hosted at CFM and organized by: Stefan T. Bromley (ICREA Professor, Universitat de Barcelona) and Jon M. Matxain (UPV/EHU and DIPC)
  Donostia-San Sebastián (Centro de Física de Materiales, CFM)

- **SOFTWARE CARPENTRY**
  June 27-29, 2016.
  Coorganizer at CFM: Iñigo Aldazabal (CSIC)
  Donostia- San Sebastián (Ignacio M. Berriola center)

- **On-Surface Synthesis**
  June 27-30, 2016.
  Coorganizers at CFM: Enrique Ortega (UPV/EHU), Celia Rogero (CSIC) and Daniel Sanchez-Portal (CSIC)
  Donostia-San Sebastián (Miramar Palace)

- **Interfacial spintronics and spin waves**
  July 18-22, 2016.
  Coorganizer at CFM: F. Sebastian Bergeret (CSIC)
  Donostia - San Sebastián (Donostia International Physics Center, DIPC)

- **Evaluación de la actividad investigadora e iniciativas de apoyo al investigador**
  July 19-20, 2016.
  Coorganizer at CFM: Ricardo Diez Muiño (CSIC)
  Donostia-San Sebastián (Miramar Palace)

- **Topological States of Matter**
  September 5-9, 2016.
  Coorganizers at CFM: F. Sebastian Bergeret (CSIC) and Vitaly N. Golovach (UPV/EHU)
  Donostia-San Sebastián (Miramar Palace)

- **Spin on Surfaces (SoS)**
  September 5-9, 2016.
  Coorganizers at CFM: Fernando Delgado (CSIC) and Nicolás Lorente (CSIC)
  Donostia-San Sebastián (Miramar Palace)

- **Workshop on Strong Coupling with Organic Molecules**
  October 19-21, 2016.
  Coorganizer at CFM: Javier Aizpurua (CSIC)
  Donostia-San Sebastián (Miramar Palace)

- **European Conference on Nanofilms: "Novel Two Dimensional materials: Synthesis, characterization and applications" (Session)**
  October 19-21, 2016
  Coorganizer at CFM: Enrique Ortega (UPV/EHU)
  Bilbao

- **Transborder Theoretical Chemistry Days**
  November 9-10, 2016.
  Coorganizer at CFM: Ricardo Diez Muiño (CSIC)
  Baiona, France

- **Técnicas de Rayos X: Análisis elementales y de estructura cristalina**
  February 18, 2016
  Organized by the Polymers and Soft Matter group of CFM
  Donostia-San Sebastián (Centro de Física de Materiales, CFM)


RESEARC
FUNDING

RESEARCH FUNDING

	2011	2012	2013	2014	2015	2016
Spanish National Plan	691514	156090	76050	838431,23	156500	1301682
International	156500	469895,62	719996	0	15600	0
Basque Government	105000	0	1350695	0	34668	0
MPC-BERC	691514	918757,39	768908,68	1316778,45	1073426	884842

(These data correspond to the overall project funding approved each year)

The following research projects were developed at CFM-MPC during 2016. These scientific projects covered a large variety of topics spread along the four research lines of the center. The projects that were running during 2016 are listed below according to the source of competitive funding, for every principal investigator (PI) at CFM:

Projects funded by the Basque Government:

Ayudas para apoyar las actividades de los grupos de investigación del sistema universitario vasco.

Solicitud IT756-13

Grupos consolidados Andrés Arnau

PI: Arnau Pino, Andrés

Ayudas para apoyar las actividades de los grupos de investigación del sistema universitario vasco.

Solicitud IT654-13

Grupos consolidados Juan Colmenero

PI: Colmenero de Leon, Juan

INF 15/14

Espectrómetro Raman de Transformada de Fourier

PI: Colmenero de Leon, Juan

Ayudas para apoyar las actividades de los grupos de investigación del sistema universitario vasco.

Solicitud IT621-13

Grupos consolidados: Enrique Ortega

PI: Ortega, Enrique

Ayudas para apoyar las actividades de los grupos de investigación del sistema universitario vasco.

Solicitud IT568-13

Grupos consolidados: Simulación de sistemas cuánticos nanoestructurados fuera del equilibrio

PI: Rubio Secades, Ángel

Projects funded by the Spanish Ministry of Economy, Industry and Competitiveness:

FIS2013-41184-P

Optoelectrónica de gaps (sub)nanométricos plasmónicos para el desarrollo de espectroscopias y microscopias aumentadas por campo

PI: Aizpurua Iriazabal, Javier

FIS2016-80174-P

Nanoplasmónica cuántica para el desarrollo del control activo en optoelectrónica, las espectroscopias aumentadas por campo y la nanoscopia

PI: Aizpurua Iriazabal, Javier

FIS2016-75862-P

Propiedades estructurales, electrónicas y magnéticas de sistemas en escala nanométrica

PI: Arnau Pino, Andrés

FIS2013-48286-C2-0-P

Electronic Processes in Surfaces and Nanostructures

PI: Ayuela Fernández, Andrés

FIS2013-48286-C2-1-P

Electronic Processes in Surfaces and Nanostructures

PI: Ayuela Fernández, Andrés

FIS2016-76617-P

Excitaciones electrónicas en superficies y nanoestructuras

PI: Ayuela Fernández, Andrés

MAT2013-48246-C2-2-P

Efecto del procesamiento sobre las propiedades ópticas de vidrios y vitrocerámicos con aplicaciones fotónicas

PI: Balda, Rolindes

FIS2014-55987-P

Transporte de espín en estructuras hibridas: metales. Superconductores, semiconductores, grafeno y aislantes topológicos

PI: Bergeret Sbarbaro, Fernando Sebastián

MAT2015-63704-P

De las nano-partículas blandas unimoleculares a los nano-compuestos totalmente polímericos

PI: Colmenero de León, Juan

FIS2016-76471-P

Transferencia de energía en la interacción y dinámica de átomos y moléculas en superficies

PI: Diez Muiño, Ricardo

FIS2013-48286-C2-2-P

Reactividad, propiedades electrónicas y estructurales de sistemas complejos

PI: Juaristi Olidén, Joseba Iñaki

MAT2015-66888-C3-2-R

Magnetismo en la nanoescala: explorando nuevas rutas (Física de dispositivos de spin)

PI: Lorente Palacios, Nicolás

MAT2013-46593-C6-4P

Híbridos covalentes en superficies

PI: Ortega Conejero, Enrique

MAT2016-78293-C6-5-R

Nanoestructuras moleculares funcionales para dispositivos optoelectrónicos: Guiando reacciones en superficies

PI: Rogero Blanco, Celia

FIS2013-43130-P

Efectos dinámicos de correlación en transporte electrónico y térmico

PI: Rubio Secades, Ángel

FIS2013-46159-C3-3-P
Desarrollos fundamentales en la simulación y caracterización de procesos dinámicos fuera del equilibrio en sistemas moleculares: materiales para aplicaciones energéticas
PI: Rubio Secades, Ángel

FIS2016-79464-P
Transporte Electrónico, Térmico, y de Espín con la Teoría de Funcionales de Densidad
PI: Rubio Secades, Ángel

MAT2013-46593-C6-2-P
Teoría de propiedades electrónicas de híbridos covalentes en superficies
PI: Sánchez Portal, Daniel

RTC-2016-5681-7
Spanish initiative for electronic simulations with thousands of atoms: Código abierto con garantía y soporte profesional, SIESTA pro
PI: Sánchez Portal, Daniel

MAT2016-78293-C6-4-R
Teoría de nanoestructuras moleculares funcionales para dispositivos optoelectrónicos
PI: Sánchez Portal, Daniel

MAT2013-46593-C64-P
Híbridos covalentes en superficies
PI: Vitali, Lucia

Projects funded by CSIC

i-COOP LIGHT 2015CD0010
Plasmónica cuántica activa en nanoantenas metálicas
PI: Aizpurua Iriazabal, Javier

i-LINK1065
Interface processes in layered organic donor-acceptor architectures
PI: Schiller, Frederik Michael

Projects funded by programs of the European Union:

ERC (Advanced-grant), Grant agreement number 267374, FP7-IDEAS-ERC
DYNAMO — Dynamical processes in open quantum systems: pushing the frontiers of theoretical spectroscopy
PI: Rubio Secades, Ángel

FP7-ICT-2013-C, Grant agreement number 618082
ACMOL — Electrical spin manipulation in electroACtive MOLecules
PI: Rubio Secades, Ángel

COST Action CM1204
XUV/X-ray light and fast ions for ultrafast chemistry (XLIC)
PI: Rubio Secades, Ángel

COST Action MP1306
Modern Tools for Spectroscopy on Advanced Materials: a European Modelling Platform
PI: Rubio Secades, Ángel

H2020-INFRAIA-2014-2015, Grant agreement number 654360
NFFA-EUROPE — Nanoscience foundries and fine analysis for Europe
PI: Rubio Secades, Ángel

H2020-NMP-2014-2015, Grant agreement number 646259
Modelling stability of organic phosphorescent light-emitting diodes
PI: Rubio Secades, Ángel

ERC (Advanced-grant), Grant agreement number 694097
QSpec-NewMat — Quantum Spectroscopy: exploring new states of matter out of equilibrium
PI: Rubio Secades, Ángel

Joint Transnational Call 2015
Trans2DTMD — Theoretical investigation of electronic transport in functionalized 2D transition metal dichalcogenides
PI: Rubio Secades, Ángel

FP7-ICT-2013.9.7 - FET Proactive, Grant Agreement number 610446
PAMS — Planar atomic and molecular scale devices
PI: Sánchez Portal, Daniel


TRANSFER
KNOWLEDG

TRANSFER OF KNOWLEDGE

TRANSFER OF KNOWLEDGE

The world-class research carried on at CFM has direct impact in society through different channels:

Transfer of knowledge

CFM is committed to give access to all the know-how and technologies resulting from its scientific activity. Both well established companies and young start-ups have the opportunity to exploit this knowledge through licensing, with continuous and direct support from the experts which have developed it in the first place. This approach has proven to be an efficient and reliable way of transferring information to the companies for its immediately use as part of innovative products and processes.

Applied & Industrial Research

CFM carries on collaborative, goal-oriented research with several industrial partners, from large international corporations to SMEs (see Projects Section). This research activity has a sharp focus on innovation, to which CFM contributes with the fundamental insight in the properties of materials. As an example of the quality of its Applied Research, CFM has been awarded with the First Prize in the first Call of the Inspire Program during May 2016.

Facilitating Entrepreneurship and Innovation.

Enhancing the competitiveness of our local economy and offering new career paths to our young researchers is one of the major concerns at CFM. This is the ultimate reason why, in collaboration with BIC Berrilan, the Center for Companies and Innovation in the province of Gipuzkoa, CFM has supported the development of several spin-off projects which are challenging the market with products and processes derived directly from the research developed in the Center, offering new job opportunities to the new cohorts of PhDs. So far, CFM holds a portfolio of three projects:

BIHURCRYSTAL

www.bihurcrystal.com

BIHURCRYSTAL provides technology for ultra-high vacuum environments (scientific infrastructure and space applications) and new materials for research, from monocrystaline samples to graphene or topological insulators. BIHURCRYSTAL has earned both Manuel Laborde and Toribio Echeberria Prizes in 2012 and 2013, respectively, attracted investment from SPRI CAPITAL RIESGO and important competitive funding from programs such as RETOS COLABORACION and NEOTEC. As of 2015, the company employs six Doctors and one technician, all former students of CFM and ICMM (Instituto de Ciencia Materiales de Madrid).

MATERIALS EVOLUTION

(http://www.etsf.eu/materials_evolution)

MATERIALS EVOLUTION focuses in applying theoretical modeling and simulation methods for accelerating the development of new materials. The initiative, awarded with Manuel Laborde prize in 2015, is supported by the European Theoretical Spectroscopy Facility, led by Angel Rubio from CFM, and runs in parallel with counterparts in Sweden and Belgium, aiming to provide a service with coverage over the whole European Region.

BASKRETE ENERGY

The most recent project at CFM is focused in exploring the potential of concrete and cement-based materials for energy storage applications. The project is backed up by the experience of the BASKRETE group, which congregates a multidisciplinary group of experts in the area of Science of Cements from CFM-MPC, UPV/EHU, TECNALIA and POLYMAT.

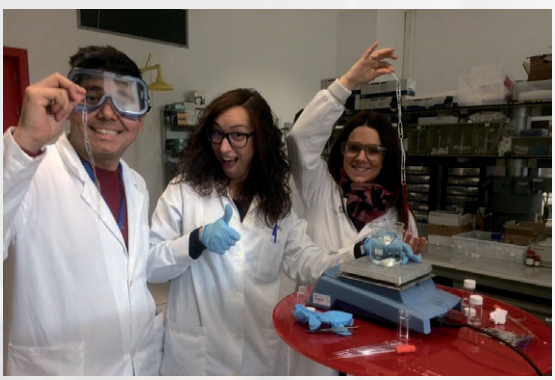
OUTREAC
ACTIVITIE

OUTREACH ACTIVITIES

OUTREACH ACTIVITIES

CFM is developing a broad program of activities aimed at bringing the excitement of science to society and especially to young people. Researchers at CFM are fully committed to spread the activities in the Center with society at many different levels. Some of the activities where CFM staff participated during 2016 follows:

High School Visits



Generating scientific vocation is one of the main goals of the outreach strategic program of the CFM. Since 2013, together with DIPC (Donostia International Physics Center) we have carried out a program of visits where both centers open their doors to high schools and other school center´s students, approximately, every two weeks during the academic year.

Besides visiting our facilities, we offer students the opportunity to directly interact with our PhD students, post-doc researchers, professors and other scientific staff, which we believe is a unique way to learn what researching is really about.

This year, CFM and DIPC have had the pleasure to host a total of 362 students from 14 schools, with more than 15 top line researchers involved in the visits.

January	February	March	April
Urretxu Zumarraga Ikastola (Zumarraga, Gipuzkoa)	**Arratia BHI** (Igorre, Bizkaia)	**Urola Garaiko Lanbide Eskola** (Zumarraga, Gipuzkoa) **Bidebieta BHI** (Donostia, Gipuzkoa)	**Padre Moret Irubide BHI** (Pamplona, Navarra) **3º Ciencia y Tecnologia de los Alimentos** (UPV/EHU) **Peñaflorida/Usandizaga BHI** (Donostia, Gipuzkoa)
May	**July**	**November**	**December**
Arrasate BHI (Arrasate, Gipuzkoa) **Lekaroz BHI** (Lekaroz, Navarra)	**Summer Maths**	**AEG ikastetxea** (Donostia, Gipuzkoa) **Bergarako Aranzadi Ikastola** (Bergara, Gipuzkoa)	**Erain** (Donostia, Gipuzkoa) **Axular Ikastola** (Donostia, Gipuzkoa)

Lanaldi program

Lanaldi program, organized by "Fundación Novia Salcedo", provides students a unique opportunity to interact with active professionals, allowing the students to spend a day with such professionals in their working places. It is a great chance to get a real perspective of what working really is about in different areas of expertise.

Following this program, last year a student from Fray Juan de Zumarraga high school (Durango) joined the spectroscopy at atomic scale group and shared a day at CFM with Lucia Vitali (Ikerbasque professor, group leader) and Alexander Correa (PhD student).

www.lanaldi.es

11/04/2016

XVI Science Week (UPV/EHU)

Between the 3rd and 5th of November 2016, CFM together with the Donostia International Physics Center (DIPC) and CIC nanoGune, joined the UPV/EHU's week of science with a stand at the Kursaal Palace in San Sebastián. In the "Exploring the tiny" stand, Master and PhD students, as well as post-doctoral researchers of the 3 centers, were involved in experiments and presentations to show the basis and applications of nanoscience and other counter-intuitive phenomena to school groups and to the average citizen. They also demonstrated how sophisticated scientific machines work, such as the Atomic Force Microscope (AFM) used to research in the field of atomic-scale surface Physics.

Kursaal Palace, Donostia/San Sebastián
3-5/11/2016

FOTCIENCIA13

FOTCIENCIA is a photography contest organized yearly by CSIC (Consejo Superior de Investigaciones Científicas) and FECYT (Fundación Española para la Ciencia y la Tecnología) in collaboration with Jesús Serra foundation. The aim of this initiative is to bring science closer to the society inviting researchers as well as citizens to participate in two categories: macro and microscopic photography.

In its 13th edition, from the 700 participating pictures, 49 photographs were selected to form part of an

exhibition that went over the country. CFM organized the exhibit in Donostia/San Sebastián showing the amazing artistic as well as scientific contribution acknowledged by the citizenship.

Andrestegi Hall, Carlos Santa Maria center UPV/EHU
15-31/03/2016

CFM as part of *Mestizajes Program* organized by DIPC

Besides traditional forms of knowledge, scientific staff at CFM also explores alternative spaces lying at the boundaries among different disciplines. *Mestizajes* is a program launched by theDIPC Foundation that bridges the gap between artistic, literary, social and scientific branches of the humanities. CFM joins this effort through Gustavo Schwartz, a tenured scientist from CSIC.

Presentation of the book "The interview"
"*The interview*" is a stage play written together by Luisa Etxenike and CFM physicist and writer Gustavo Ariel Schwartz in a novel trans-disciplinary collaboration. This joint writing work was done in the framework of *Mestizajes*. In 2016, the publication of the play in a bilingual edition (Spanish/English) by the editorial "El Gallo de Oro" was presented in San Sebastián, Bilbao and Madrid.

San Telmo Museoa, Donostia/San Sebastián
19/02/2016

Realidad Conexa (Cápsulas audiovisuales)
"Realidad Conexa" is a collection of 8 audiovisual capsules dealing with intuition and reasoning, mixing and matching science, art and literature. This project is also part of the program *Mestizajes* and has been supported by DIPC (Donostia International Physics Center). Gustavo Ariel Schwartz, together with Ana Montserrat, the many times awarded director, explored the connections among different fields of knowledge in a novel and contemporary way.

Presented in Passion For Knowledge 2016, Donostia/San Sebastián

See the video series scanning this code

Outreach talks

“De asesinatos, detectives y teoremas. Matemáticas en la novela negra”
Raul Ibáñez Torres (Mathematics professor at UPV/EHU; science outreach in public media)

From Edgar Allan Poe to the Millennium best seller of Stieg Larson, the crime and mystery novel is probably the genre with greater presence of mathematics, perhaps just after science fiction. In this talk Raul Ibáñez, the celebrated mathematics professor, analyzed the relation between Pythagoras and crime novels, the parallelism between a mathematic and a police research, or the role of detectives versus researchers, being mathematics the fundamental clue of the conspiracy.

Organized by: Gustavo Ariel Schwartz (Tenured scientist at CFM, CSIC)
Biblioteca Central- Donostia Kultura, Donostia/ San Sebastián
17/05/2016

“Mestizaje Transdisciplinar. La especialización es para los insectos.”
VII Brilliant Minds Congress
“El Ser Creativo” is a company focused in the search of ideas that may change the world. With a multidisciplinary approach, they organize events, such as the congress “Brilliant minds”, where national and international experts are gathered to discuss different areas of expertise, including arts and sciences. In this context, CFM researcher Gustavo Ariel Schwartz presented the talk “Mestizaje Transdisciplinar. La especialización es para los insectos”.

Madrid
13-14/10/2016

See the talk
scanning this code

DSS2016 Donostia /San Sebastián European Capital of Culture

In 2016 Donostia/San Sebastián was honored to be chosen as the European Capital of Culture. The city has been devoted to the task, offering a wide variety of activities that cover the whole year, bringing culture insights into public scene. Science has played a key role as a part of the cultural background of the city. In this matter, CFM has actively collaborated with the events at DSS2016 participating in talks, meetings and other activities, the most notable being the following ones.

Urbanzientzia (Urbanscience)
Organized by TEKNAHI

"Waves of energy" sums up the "soul" of the "San Sebastián 2016" candidature in a clear message: people and movements of citizens are the real driving force behind transformations and changes in the world. Urbanscience was part of these waves of energy. It consisted of a series of activities organized for one day right on the street where citizens could directly participate and interact with researchers with a wide variety of proposals. CFM participated in two activities:

- Hands-on stand entitled "Inspired by the little secrets of nature" together with DIPC and CIC nanoGUNE.
- Outreach talk "Molekulak ikusi nahi zituen kuxkusero baten istorioa, the curious boy who wanted to look into the molecules". Talk in a tale format with Javier Aizpurua, CFM´s director, as the storyteller.

Iztueta Street, Donostia/ San Sebastián
21/05/2016

See the talk scanning this code

"Desafíos/Erronkak/ Challenges"
Organized by Jakiunde

This meeting was organized by Jakiunde and DSS2016, with the collaboration of museum San Telmo, in the framework of the initiative "Desafíos/Erronkak" to analyze and show some challenges that nowadays society faces. During this edition of "Challenges", the possibilities of new materials were explored. In this context, CFM participated with two outreach talks: "Nanofotónica-Nanophotonics" by Javier Aizpurua and "Resembling nature: nanotechnology of individual macromolecules" by Josetxo Pomposo.

San Telmo museum, Donostia/San Sebastián
04/05/2016

Awards

Pedro Miguel Echenique

Professor of the University of the Basque Country (UPV/EHU), member of CFM, and President of Material Physics Center (MPC) and Donostia International Physics Center (DIPC)

Gold Medal of Navarra/*Medalla de oro de Navarra*
03/12/2016

The Government of Navarra has awarded the Gold Medal of Navarra to Pedro Miguel Echenique. The award, the most important of Navarra´s Government, recognizes the "intellectual, scientific and human dimension" of his research and outreach works in the field of physics.

Dr. Honoris causa Aalto University (Finland)
07/10/2016

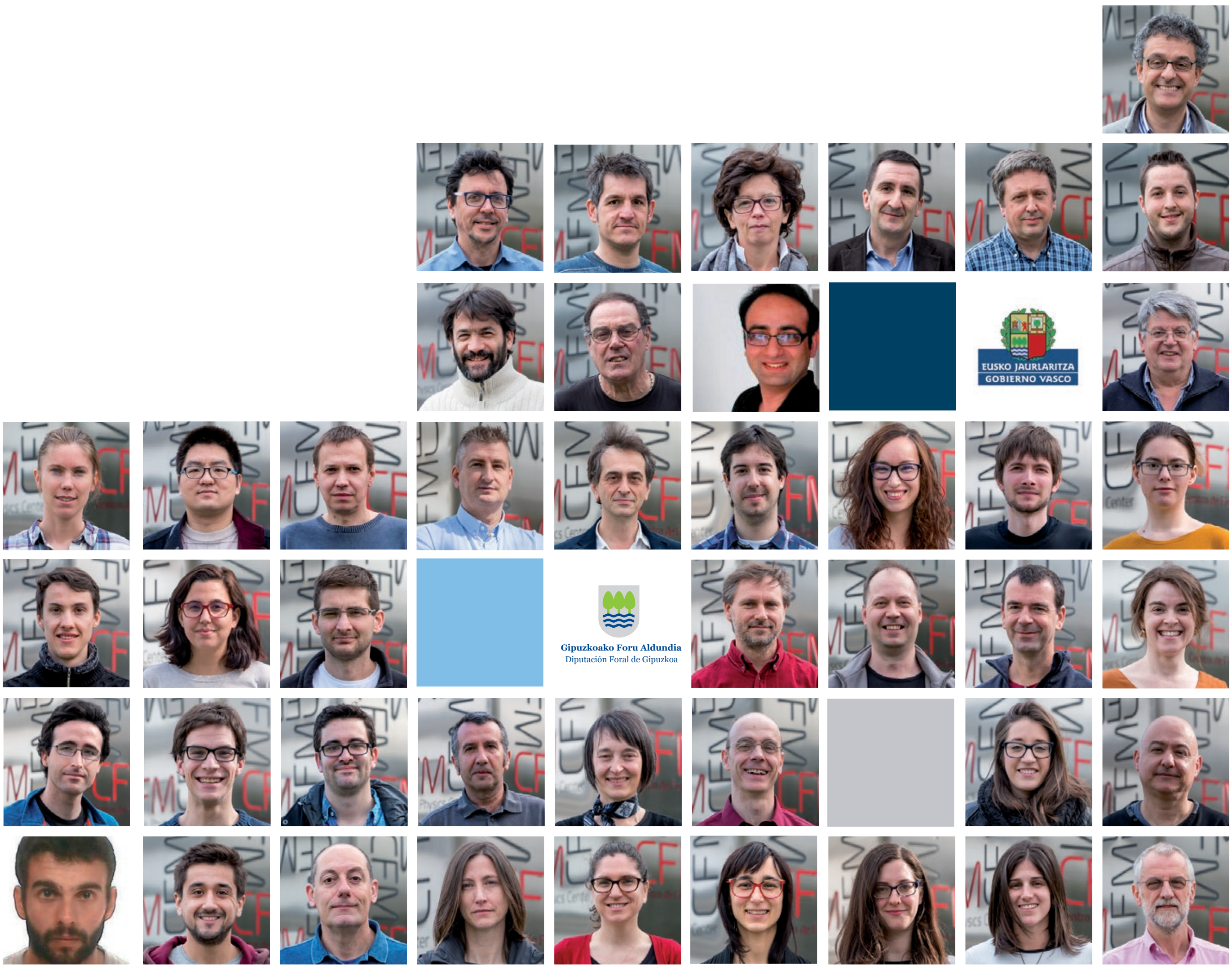
Pedro Miguel Echenique has been invested Doctor Honoris Causa in Technology at the Aalto University, in Finland. This distinction, which has been conferred every two years over the last 80 years by the Aalto University Schools of Technology, has been awarded to 10 eminent personalities from the world of science, technology and society, in addition to Professor Echenique.

Ángel Rubio

Medal of the Spanish Royal Society of Physics/ *Medalla de la Real Sociedad Española de Física*
17/10/2016

The Spanish Royal Society of Physics has awarded the medal of the institution to Ángel Rubio, Professor of the University of the Basque Country (UPV/EHU), leader of the Nano-bio Spectroscopy Group, member of CFM and director of the Theory department at the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg, Germany. This is the second time that the Spanish Royal Society of Physics recognizes his activity. In 1991, Prof. Rubio was given the Young Investigator Award.

THE ELEMENTS OF CFM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