ACTIVITY REPORT 2015

CFM
Centro de Física de Materiales
Materials Physics Center

Centro de Física de Materiales
Materialen Fisika Zentroa
Materials Physics Center

CSIC

Universidad del País Vasco
Euskal Herriko Unibertsitatea

MPC
Materials Physics Center
BERC

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MPC
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Summary

Introduction/Foreword

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. 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-MPC is located at Ibaeta Campus in Donostia – San Sebastian, at the very core of a thrilling research community focused in 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-MPC plays a central role, representing its founding institutions and hosting a stable critical mass of world-class research groups focused in fundamental materials science. CFM-MPC activity is developed by a core of scientist, 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-MPC in four main research lines, (i) Chemistry of complex systems, (ii) Electrons in Solids, (iii) Photonics, and (iv) Soft matter, has proven to be an efficient scientific framework, where experimentalist and theoreticians with different backgrounds exchange ideas and pursuit challenging scientific goals, but also where students receive up-to-date training and have the chance to interact with world-class researchers.

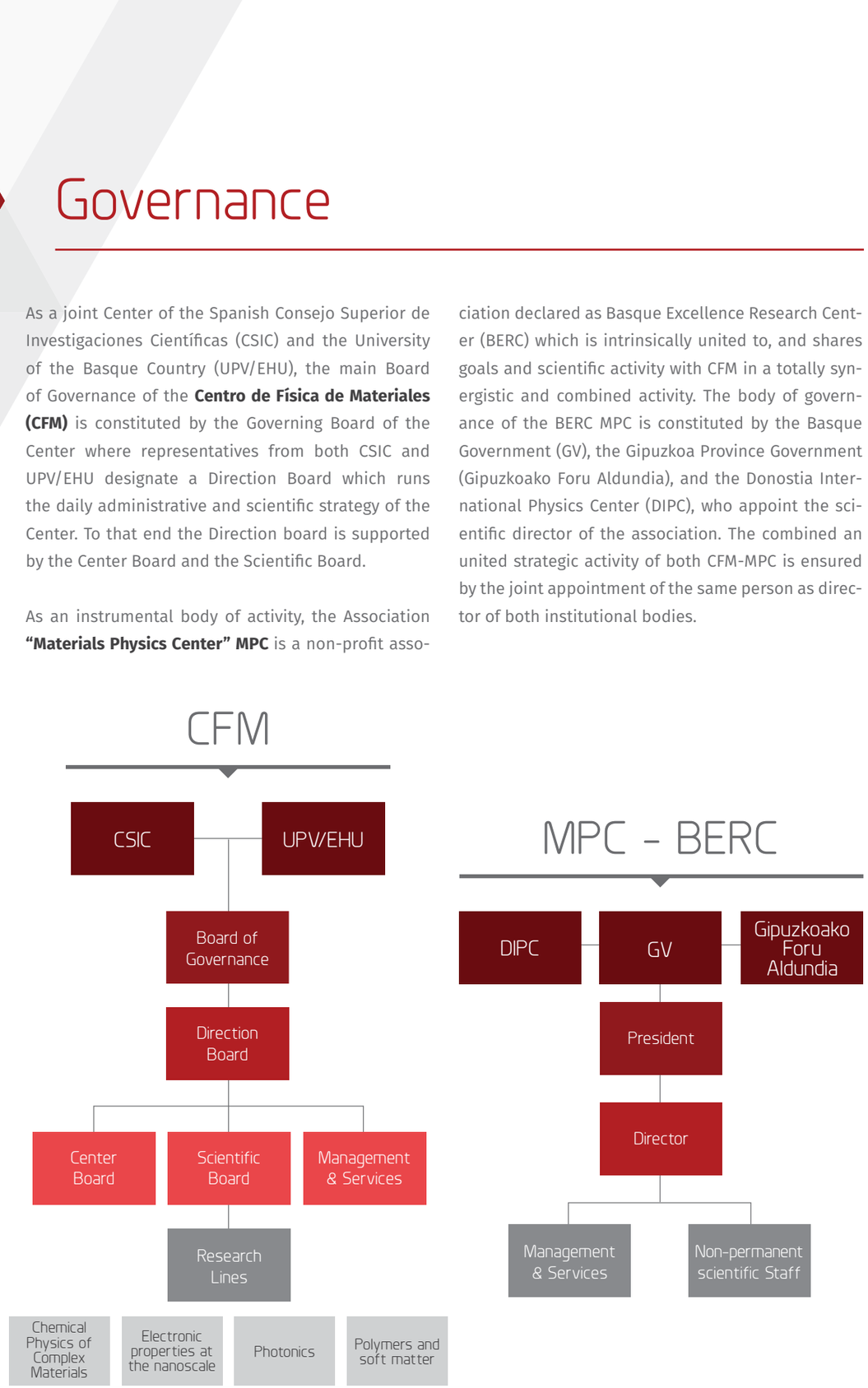
Despite CFM-MPC's orientation towards fundamental research, cooperation with industry is an important goal that ensures that our society also benefits from our activity. We are especially proud of the spin-off and start-up initiatives launched during 2015, which provide some of our young researchers with new career perspectives and bring the entrepreneurial culture into the daily activities of the center, multiplying the opportunities for cooperation.

Along 2015 Javier Aizpurua has taken the baton from Ricardo Díez Muiño at the Head of CFM-MPC. Ricardo's hard and relentless work during the last four years has allowed for preserving the high-quality working environment as well as meeting the ambitious scientific goals of the center during the last years, despite the difficult financial situation. Thanks to the constant effort of the whole human team, CFM-MPC 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.

Governance

As 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 **Centro de Física de Materiales (CFM)** is constituted by the Governing Board of the Center 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.

As an instrumental body of activity, 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 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 an united strategic activity of both CFM-MPC is ensured by the joint appointment of the same person as director of both institutional bodies.



Human Resources in 2015

DIRECTION BOARD

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

MANAGEMENT

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

COMPUTING SERVICES

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

TECHNICAL SUPPORT

Silvia Arrese-Igor Irigoyen, Technician R+D+I, CSIC
Luis Botana Salgueiros, Technician R+D+I, CSIC
María Isabel Asenjo Sanz, Technician, MPC
Amaia Iturrospe Ibarra, Technician, MPC
Juan José Gil Miranda, Technician, CSIC
Josu Atxa Noguero, Student, MPC (since march 2015, until november 2015)
Tamara Molina Rola, Student, MPC (since november 2015)

Research line:

CHEMICAL PHYSICS OF COMPLEX MATERIALS

Staff

Maite Alducin Ochoa, Tenured Scientist, CSIC
Andrés Arnau Pino, University Professor, UPV/EHU
Ricardo Díez Muiño, Tenured Scientist, CSIC
Iñaki Juaristi Oliden, Associate Professor, UPV/EHU
Jorge Lobo Checa, Tenured Scientist, CSIC (until september 2015)
Enrique Ortega Conejero, University Professor, UPV/EHU
Celia Rogero Blanco, Tenured Scientist, CSIC
Daniel Sánchez Portal, Research Scientist, CSIC
Frederik Michael Schiller, Tenured Scientist, CSIC
Ivo Souza, Ikerbasque Professor , UPV/EHU
Lucia Vitali, Ikerbasque Professor, UPV/EHU

Ikerbasque Fellows

Martina Corso, UPV/EHU
Fernando Delgado Acosta, UPV/EHU

Postdoctoral Researchers

Pedro Brandimarte Mendonça
Jens Brede
Mads Engelund
Daniel Gosálbez
Maxim Ilin
Stepan Tsirkin
Guillaume Vasseur

PhD Students

Mikel Abadía Gutiérrez
Marc Barbry
Ana Barragán Duran
Alexander Correa Aristizabal
Iker Gallardo Arrieta
Oihana Galparsoro Larraza
Natalia Koval
Ivor Lončaric
Ana Magaña Vicandi
Federico Marchesin
Flavio Matias
Nestor Merino Diez
Moritz Mueller
Ahmed Mohamed Abdel Azim Nosir
Ignacio Piquero Zulaica

Research line:

ELECTRONIC PROPERTIES AT THE NANOSCALE

Staff

Andrés Ayuela Fernández, Research Scientist, CSIC
Aitor Bergara Jauregi, Associated Professor, UPV/EHU
Sebastián Bergeret Sbarbaro, Tenured Scientist, CSIC
Pedro Miguel Echenique Landiribar, University Professor, UPV/EHU
Nicolás Lorente Palacios, Research Scientist, CSIC
José Maria Pitarke de la Torre, University Professor, UPV/EHU
Ángel Rubio Secades, University Professor, UPV/EHU
Evgeni V. Tchoulkov, University Professor, UPV/EHU

Ikerbasque Fellow

Vitaly Golovach, UPV/EHU

Postdoctoral Researchers

Ali Abedi
Jhon Wilfer González Salazar
Hannes Simon Hübener
Seymur Jahangirov
Elham Khosravi
Francois Xabier Konschelle
Ilya Nechaev
Marta Pelc

PhD Students

Tomás Alonso Lanza
Miguel Borinaga Treviño
Alison Crawford Uranga
Mehdi Farzanehpour
Alba Pascual Gil

Research line:

PHOTONICS

Staff

Javier Aizpurua Iriazabal, Research Professor, CSIC
Rolindes Balda de la Cruz, University Professor, UPV/EHU
Joaquín Fernández Rodríguez, University Professor, UPV/EHU
Yury Rakovich, Ikerbasque Professor, UPV/EHU
Alberto Rivacoba Ochoa, University Professor, UPV/EHU
Nerea Zabala Unzalu, Associate Professor, UPV/EHU

Postdoctoral Researchers

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Dzmitry Melnikau
Christos Tserkezis
Yao Zhang

PhD Students

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Andrea Konecna
Tomas Neuman
Mohamed Ameen Poyli
Mikolaj Schmidt
Mattin Urbieta Galarraga

Research line:

POLYMERS AND SOFT MATTER

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

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Ewa Golas
Federica Loverso
Paula Angela Malo de Molina Hernández
Ana Lucia Rodríguez Garraza

PhD Students

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Izaskun Combarro Palacios
Thomas Gambino
Marina González Burgos
Guido Goracci
Natalia Gutiérrez Pérez de Eulate
Stefan Holler
Alejandro Latorre Sánchez
Gerardo Martínez Rugeiro
Manuel Monasterio Jaqueti
Lucía Ortega Alvarez
Jon Rubio Cervilla

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
Rubén González Moreno, Postdoctoral Researcher, BIHURCRYSTAL (spin-off)
Alejandro Miccio, Postdoctoral Researcher, BIHURCRYSTAL (spin-off)

Visitors

CFM received around 70 short- and long-term visiting researchers during 2015.

Representative Research Activities

› Chemical physics of complex materials team

X-ray photoemission analysis of clean and carbon monoxide-chemisorbed platinum(111) stepped surfaces using a curved crystal

A.L Walter, F. Schiller, M. Corso, L.R. Merte, F. Bertram, J. Lobo-Checa, M. Shpilin, J. Gustafson, E. Lundgren, A. X. Bríon-Rios, P. Cabrera-Sanfelix, D. Sánchez-Portal, E. Ortega

Nature Communications 6, 8903 (2015)

Surface chemistry and catalysis studies could significantly gain from the systematic variation of surface active sites, tested under the very same conditions. Curved crystals are excellent platforms to perform such systematics, which may in turn allow to better resolve fundamental properties and reveal new phenomena. This is demonstrated here for the carbon monoxide/platinum system. We curve a platinum crystal around the high-symmetry (111) direction and carry out photoemission scans on top. This renders the spatial core-level imaging of carbon monoxide adsorbed on a 'tunable' vicinal surface, allowing a straightforward visualization of the rich chemisorption phenomenology at steps and terraces. Through such photoemission images we probe a characteristic elastic strain variation at stepped surfaces, and unveil subtle stress-release effects on clean and covered vicinal surfaces. These results offer the prospect of applying the curved surface approach to rationally investigate the chemical activity of surfaces under real pressure conditions.

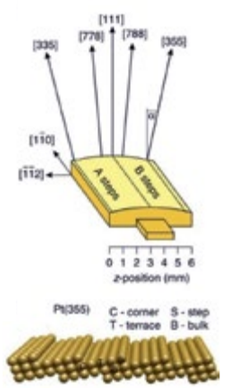


Figure:

Schematic representation of the Curved Crystal Concept. A monocrystalline sample with atom-defined curved surface allows accessing different crystalline orientations, including exotic ones.

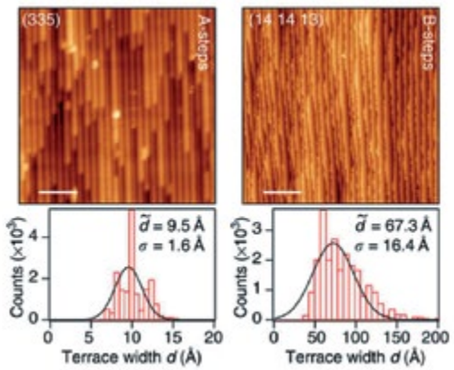


Figure:

STM images at selected surface orientations, showing step lattice variations at the atomic scale.

Electronic Properties at the Nanoscale

Pb/InAs Nanowire Josephson Junction with High Critical Current and Magnetic Flux Focusing

J. Paajaste, M. Amado, S. Roddaro, FS. Bergeret, D. Ercolani, L. Sorba, F. Giazotto

Nano Letters 15, 1803 (2015)

Josephson junctions and coherent quantum transport have been attracting interest in recent years due to the development of modern nanofabrication techniques, which enable the fabrication of nanoscale hybrid superconducting devices in a broad range of design and materials. Josephson junctions realized with semiconductor nanowires (NWs) have shown a high potential in different types of nanoscale devices demonstrating, for example, tunable supercurrents, the supercurrent reversal, and the suppression of supercurrent by hot electron injection. NWs have also been used for superconducting quantum interference devices (SQUIDs) and tunable Cooper pair splitters. Benefits of using NWs include the tunable charge density by means of a gate voltage that in turn tunes the supercurrent. Yet, small dimensions of NWs also make them a promising choice for studying fundamental phenomena such as the quantum interference and Majorana fermions.

In this collaborative work, carried out by the groups led by F. Giazzotto (NEST, CNR - Scuola Normale Superiore di Pisa, Italy and S. Bergeret (CFM, CSIC – UPV/EHU, Spain) we have successfully fabricated mesoscopic Pb/InAs-NW/Pb Josephson junctions with ~100 nm interelectrode spacing by room-temperature Pb evaporation. Devices show excellent properties in terms of a high critical current exceeding 600 nA and an observable Josephson current at temperatures up to 4.5 K and magnetic fields up to 0.3 T. Superconductivity is observed in the electrodes up to ~7 K. Unlike the expected behaviour in narrow junctions where the width is smaller than the magnetic length, we observe a marked diffraction pattern of the critical current as a function of the magnetic field which can be explained by a strong magnetic flux focusing provided by the Pb electrodes.

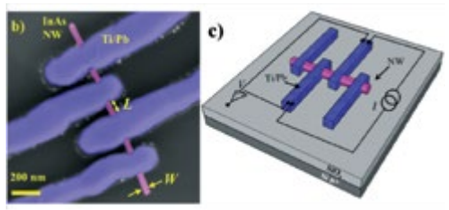


Figure:

Left) Electron micrograph (false colour) of the InAs-based Josephson junction

Right) Schematic description of the device.

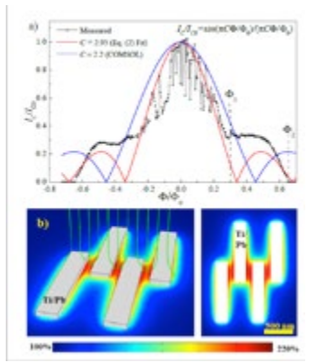


Figure:

Top) Normalized critical current versus magnetic flux, showing the Fraunhofer patterns.

Bottom) Simulation showing the strength of perpendicular magnetic flux as a function of position.

Photonics

Nano-optics of molecular-shunted plasmonic nanojunctions

F. Benz, Ch. Tserkezis, L.O. Herrmann, B. de Nijs, A. Sanders, D.O. Sigle, L. Pukenas, S.D. Evans, J. Aizpurua, and J.J. Baumberg

Nano Letters 15, 669 (2015)

The interplay of photons and electrons in a molecule is at the base of modern molecular optoelectronics, however to access the transport properties of molecules at very high AC frequencies is not possible with the current capabilities of electronics. A joint recent study between researchers from Cambridge and CFM-MPC analyses the optical response of a plasmonic metallic cavity shunted by molecular linkers as a monitor that provides valuable information about this ultrafast transport regime. Furthermore, the optical methodology introduced in this work can determine the number of molecules involved in the transport through a cavity, as well as their unitary conductance. The results obtained by this collaborative effort thus impacts the field of molecular devices for optoelectronics.

Metallic junctions provide a fantastic platform to test molecular transport properties. When a bias between two metallic electrodes is applied the current through the junction is mainly determined by the distance between the two metallic interfaces, as well as by the intrinsic transport properties of the material within the junction. In a collaboration with the Nanophotonics Centre in Cambridge (U.K.), researchers from the Center for Materials Physics in Donostia-San Sebastián have explored the optical fingerprints of conductivity in molecular- shunted plasmonic junctions.

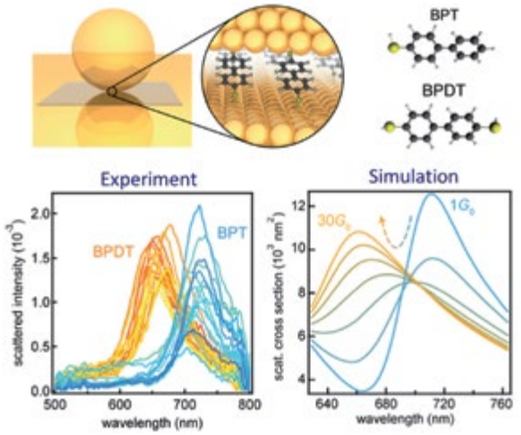


Figure:

(Top) Schematics of a plasmonic junction formed by a metallic nanoparticle on a metallic surface shunted by a self-assembled monolayer of BPT and BPDT molecules.

(Bottom) Experimental and theoretical spectral blue-shift of the plasmonic cavity when the non-conductive molecules (BPT) are substituted by conductive ones (BPDT).

In this work, the optical response of a cav-

ity plasmon was monitored as a function of the molecular conductance across the cavity formed by a nanoparticle deposited on a metallic surface (see schematics of the system on top of the figure). To progressively change the conductance at the cavity, two different species of molecular linkers were used: (i) a conductive biphenyl-4-4'-dithiol (BPDT) molecule with the thiols linked to both metallic interfaces forming the cavity, and (ii) a biphenyl-4-thiol (BPT) molecule where one of the thiol connections of the BPDT is removed, preventing conduction through it. The chemical structure of both molecules can be observed on the top of the figure, on the right hand side. As the ratio of the conducting molecules within the cavity is progressively modified with respect to the nonconducting ones, a screening of the cavity plasmon is produced, that progressively modifies the capacitance of the bonding plasmon formed at the cavity, and thus modifying its resonance wavelength. This behavior had been predicted by researchers at the CFM, and has been now corroborated experimentally by the researchers in Cambridge led by Prof. J. J. Baumberg. The results show an experimental blue-shift of the screened plasmon of about 60 nm, as observed in the figure attached (bottom, left), when all the nonconductive molecules are substituted by conducting ones. According to the numerical calculations developed at the CFM in San Sebastian, a conductance of 30 G_o across the cavity (with G_o the quantum of conductance) is necessary to produce the observed blue-shift. By applying a simple circuit theory model, where the spectral shift can be associated with the reduction of the capacitance of the screened charge of the plasmon, the calculated conductance provided an estimation of the number of conducting molecules in the cavity (around 200 BPDT), as well as of the conductance per molecule (about 0.17 G_o).

To obtain information on the high-frequency transport properties of molecular-shunted junctions by optical means provides new venues to explore important constructs in optoelectronics, as well as to reach regimes of transport not accessible by other means.

› Polymers and Soft Matter

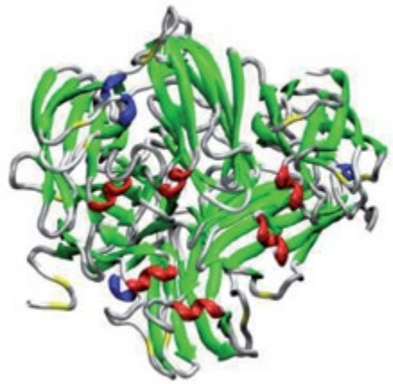
Efficient Synthesis of Single-Chain Globules Mimicking the Morphology and Polymerase Activity of Metalloenzymes

A. Sanchez-Sanchez, A. Arbe, J. Kohlbrecher, J. Colmenero, J. Pomposo

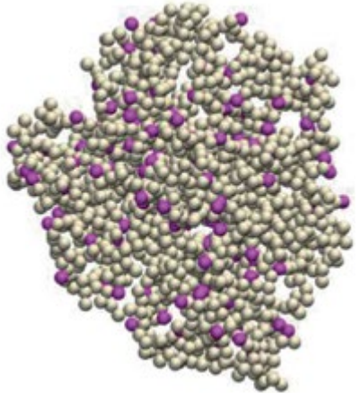
Macromolecular Rapid Communications 36, 1592 (2015)

About one-third of all enzymes known so far are metalloenzymes containing metal ions which are directly bound to the protein or to prosthetic groups (non-amino acid portions required for enzyme function firmly bonded to the protein). Recently, it has been discovered that metalloenzymes (laccase, horseradish peroxidase, hemoglobin) show polymerase activity, i.e., they catalyze the controlled radical polymerization of water soluble vinyl-type monomers. We were intrigued by this discovery and, especially, by the potential feasibility of designing bioinspired synthetic nano-objects having metalloenzyme mimicking properties for the controlled synthesis of water-soluble polymers. In this sense, endowing unimolecular soft nano-objects with biomimetic functions is attracting significant interest in the emerging field of single chain technology.

Hence, inspired by the compartmentalized structure and polymerase activity of metalloenzymes we have designed, synthesized and characterized copper-containing compact nano-globules endowed with metalloenzyme mimicking characteristics towards controlled synthesis of water-soluble polymers and thermoresponsive hydrogels. To our best knowledge, this has been the first report of water-soluble polymers and thermoresponsive hydrogels synthesized by metal-containing single chain globules. When compared to metalloenzymes, artificial nano-objects endowed with metalloenzyme mimicking characteristics offer increased stability against thermal changes and reduced degradability by hydrolytic enzymes.



Lacase enzyme



Single-chain globule

Research output

We provide in the following some representative indicators of the research activity of CFM-MPC during 2015.

AVERAGE IMPACT FACTOR OF THE CENTER **5,127**

NUMBER OF ARTICLES **173**

Among all the scientific articles written by researchers at CFM-MPC in 2015, we list below a selection of them published in high impact-factor journals.

JOURNAL	Number of articles	Impact factor	Accumulated Impact factor
Nature Materials	1	36,503	36,503
Nature Nanotechnology	1	34,048	34,048
Chemical Society Reviews	1	33,383	33,383
Nature Physics	1	20,147	20,147
Nano Letters	5	13,592	67,960
ACS Nano	3	12,881	38,643
Nature Communications	2	11,470	22,940
Angewandte Chemie-International	1	11,261	11,261
Proceedings of the National Academy of Sciences of the United States of America	1	9,674	9,674
ACS Catalysis	1	9,312	9,312
Chemical Science	1	9,211	9,211
Chemistry Of Materials	1	8,354	8,354
Laser & Photonics Reviews	1	8,008	8,008
Physical Review Letters	10	7,512	75,120
Journal Of Physical Chemistry Letters	2	7,458	14,916

Among all the articles published at CFM-MPC, 79,19% of the articles (135 out 173) were published in the framework of international collaborations, showing the international dimension and positioning of the Center in the field of Materials Science.

› Publication list

1

Functionalization of Defect Sites in Graphene with RuO_2 for High Capacitive Performance

Yang F, Zhang LB, Zuzuarregui A, Gregorczyk K, Li L, Beltran M, Tollan C, Brede J, Rogero C, Chuvilin A, Knez M.

ACS Applied Materials & Interfaces 7, 20513 (2015)

2

Comparing Quasiparticle H_2O Level Alignment on Anatase and Rutile TiO_2

Sun H, Mowbray DJ, Migani A, Zhao J, Petek H, Rubio A.

ACS Catalysis 5, 4242 (2015)

3

Bipolar Conductance Switching of Single Anthradithiophene Molecules

Borca B, Schendel V, Petuya R, Pentegov I, Michnowicz T, Kraft U, Klauk H, Arnau A, Wahl P, Schlickum U, Kern K.

ACS Nano 9, 12506 (2015)

4

Epitaxial B-Graphene: Large-Scale Growth and Atomic Structure

Usachov DY, Fedorov AV, Petukhov AE, Vilkov OY, Rybkin AG, Otrokov MM, Arnau A, Chulkov EV, Yashina LV, Farjam M, Adamchuk VK, Senkovskiy BV, Laubschat C, Vyalikh DV.

ACS Nano 9, 7314 (2015)

5

Monitoring Morphological Changes in 2D Mono layer Semiconductors Using Atom-Thick Plasmonic Nanocavities

Sigle DO, Mertens J, Herrmann LO, Bowman RW, Ithurria S, Dubertret B, Shi YM, Yang HY, Tserkezis C, Aizpurua J, Baumberg JJ.

ACS Nano 9, 825 (2015)

6

The Morphology of Narrow Gaps Modifies the Plasmonic Response

Esteban R, Aguirregabiria G, Borisov AG, Wang YMM, Nordlander P, Bryant GW, Aizpurua J.

ACS Photonics 2, 295 (2015)

7

Electromagnetic Resonances of Silicon Nanoparticle Dimers in the Visible

Zywietz U, Schmidt MK, Evlyukhin AB, Reinhardt C, Aizpurua J, Chichkov BN.

ACS Photonics 2, 913 (2015)

8

Electronic Bandgap and Exciton Binding Energy of Layered Semiconductor TiS_3

Molina-Mendoza AJ, Barawi M., Biele R, Flores E, Ares JR, Sánchez C, Rubio-Bollinger G, Agraït N, D'Agosta R, Ferrer IJ, Castellanos-Gomez A.

Advanced Electronic Materials 1, 1500126 (2015)

9

Engineering Photophenomena in Large, 3D Structures Composed of Self-Assembled van der Waals Heterostructure Flakes

Krishna MBM, Man MKL, Vinod S, Chin C, Harada T, Taha-Tijerina J, Tiwary CS, Nguyen P, Chang P, Narayanan TN, Rubio A, Ajayan PM, Talapatra S, Dani KM.

Advanced Optical Materials 3, 1551 (2015)

10

Unraveling the Intrinsic Color of Chlorophyll

Milne BF, Toker Y, Rubio A, Nielsen SB.

Angewandte Chemie-International Edition 54, 2170 (2015)

11

Influence of size, shape and core-shell interface on surface plasmon resonance in Ag and Ag@MgO nanoparticle films deposited on Si/SiO_x

D'Addato S, Pinotti D, Spadaro MC, Paolicelli G, Grillo V, Valeri S, Pasquali L, Bergamini L, Corni S.

Beilstein Journal of Nanotechnology 6, 404 (2015)

12

Membrane dipole modifiers modulate single-length nystatin channels via reducing elastic stress in the vicinity of the lipid mouth of a pore

Chulkov EG, Schagina LV, Ostroumova OS.

Biochimica et Biophysica Acta- Biomembranes 1848, 192 (2015)

13

Angular distributions and rovibrational excitation of N_2 molecules recombined on N-covered Ag(111) by the Eley-Rideal mechanis

Juaristi JI, Diaz E, Bocan GA, Muino RD, Alducin M, Blanco-Rey M.

Catalysis Today 244, 115 (2015)

14

A simple, fast and highly sensitive colorimetric detection of zein in aqueous ethanol via zein-pyridine-gold interactions

Latorre Sanchez A, Pomposo JA.

Chemical communications 51, 15736 (2015)

15

Design of two-photon molecular tandem architectures for solar cells by ab initio theory

Ornso KB, Garcia-Lastra JM, De La Torre G, Himpsel FJ, Rubio A, Thygesen KS.

Chemical Science 6, 3018 (2015)

16

Advances in single chain technology

Gonzalez Burgos M, Latorre Sanchez A, Pomposo JA.

Chemical Society Reviews 44, 6122 (2015)

17

Tuning the Tensile Strength of Cellulose through Vapor-Phase Metalation

Gregorczyk KE, Pickup DF, Sanz MG, Irakulis IA, Rogero C, Knez M.

Chemistry Of Materials 27, 181 (2015)

18

Chemical Bonding of Transition-Metal Co_{13} Clusters with Graphene

Alonso-Lanza T, Ayuela A, Aguilera-Granja F.

Chemphyschem 16, 3700 (2015)

19

Assessment of Density-Functional Tight-Binding Ionization Potentials and Electron Affinities of Molecules of Interest for Organic Solar Cells Against First-Principles GW Calculations

Darghouth AAMHM, Casida ME, Taouali W, Alimi K, Ljungberg MP, Koval P, Sanchez-Portal D, Foerster D.

Computation 3, 616 (2015)

20

Design and performance characterization of electronic structure calculations on massively parallel supercomputers: a case study of GPAW on the Blue Gene/P architecture

Romero NA, Glinsvad C, Larsen AH, Enkovaara J, Shende S, Morozov VA, Mortensen JJ.

Concurrency And Computation-Practicle & Experience 27, 69 (2015)

21

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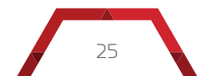

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Atomic and electronic structure of bismuth-bilayer-terminated Bi_2Se_3(0001) prepared by atomic hydrogen etching

Shokri R, Meyerheim HL, Roy S, Mohseni K, Ernst A, Otrokov MM, Chulkov EV, Kirschner J.

Physical Review B 91, 205430 (2015)

131

Vibron-assisted spin relaxation at a metal/organic interface

Droghetti A, Rungger I, Cinchetti M, Sanvito S.

Physical Review B 91, 22 (2015)

132

Quasiparticle spectrum and plasmonic excitations in the topological insulator Sb_2Te_3

Nechaev IA, Aguilera I, De Renzi V, di Bona A, Rizzini AL, Mio AM, Nicotra G, Politano A, Scalese S, Aliev ZS, Babanly MB, Friedrich C, Blugel S, Chulkov EV.

Physical Review B 91, 245123 (2015)

133

Sublattice effect on topological surface states in complex $(S_nTe)_{n>1}(Bi_2Te_3)_{m=1}$ compounds

Eremeev SV, Menshchikova TV, Silkin IV, Vergniory MG, Echenique PM, Chulkov EV.

Physical Review B 91, 245145 (2015)

134

Surface alloying and iron selenide formation in Fe/Bi_2Se_3(0001) observed by x-ray absorption fine structure experiments

Polyakov A, Meyerheim HL, Crozier ED, Gordon RA, Mohseni K, Roy S, Ernst A, Vergniory MG, Zubizarreta X, Otrokov MM, Chulkov EV, Kirschner J.

Physical Review B 92, 045423 (2015)

135

Transmission through correlated CunCoCun heterostructures

Chioncel L, Morari C, Ostlin A, Appelt WH, Droghetti A, Radonjic MM, Rungger I, Vitos L, Eckern U, Postnikov AV.

Physical Review B 92, 054431 (2015)

136

Cubic-scaling iterative solution of the Bethe-Salpeter equation for finite systems

Ljungberg MP, Koval P, Ferrari F, Foerster D, Sanchez-Portal D.

Physical Review B 92, 075422 (2015)

137

Chiral degeneracies and Fermi-surface Chern numbers in bcc Fe

Gosalbez-Martinez D, Souza I, Vanderbilt D.

Physical Review B 92, 085138 (2015)

138

Topologically confined states at corrugations of gated bilayer graphene

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

Physical Review B 92, 085433 (2015)

139

Valley Hall effect in disordered monolayer MoS2 from first principles

Olsen T, Souza I

Physical Review B 92, 125146 (2015)

140

Influence of surface electronic structure on quantum friction between Ag(111) slabs

Despoja V, Silkin VM, Echenique PM, Sunjic M.

Physical Review B 92, 125424 (2015)

141

Theory of the spin-galvanic effect and the anomalous phase shift phi(0) in superconductors and Josephson junctions with intrinsic spin- orbit coupling

Konschelle F, Tokatly IV, Bergeret FS.

Physical Review B 92, 125443 (2015)

142

Ultrafast electronic response of Ag(111) and Cu(111) surfaces: From early excitonic transients to saturated image potential

Silkin VM, Laziz P, Doslic N, Petek H, Gumhalter B.

Physical Review B 92, 155405 (2015)

143

Breaking time-reversal symmetry at the topological insulator surface by metal-organic coordination networks

Otrokov MM, Chulkov EV, Arnau A.

Physical Review B 92, 165309 (2015)

144

Variation of the character of spin-orbit interaction by Pt intercalation underneath graphene on Ir(111)

Klimovskikh II, Vilkov O, Usachov DY, Rybkin AG, Tsirkin SS, Filianina MV, Bokai K, Chulkov EV, Shikin AM.

Physical Review B 92, 165402 (2015)

145

Ab initio analysis of the topological phase diagram of the Haldane model

Ibanez-Azpiroz J, Eiguren A, Bergara A, Pettini G, Modugno M.

Physical Review B 92, 195132 (2015)

146

Ab initio molecular dynamics with simultaneous electron and phonon excitations: Application to the relaxation of hot atoms and molecules on metal surfaces

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

Physical Review B 92, 201411 (2015)

147

Termination-dependent surface properties in the giant-Rashba semiconductors BiTeX (X = Cl, Br, I)

Fiedler S, Bathon T, Eremeev SV, Tereshchenko OE, Kokh KA, Chulkov EV, Sessi P, Bentmann H, Bode M, Reinert F.

Physical Review B 92, 23 (2015)

148

Inelastic decay of electrons in Shockley-type metal-organic interface states

Tsirkin SS, Zaitsev NL, Nechaev IA, Tonner R, Hofer U, Chulkov EV.

Physical Review B 92, 235434 (2015)

149

Electronic and spin structure of a family of Sn-based ternary topological insulators

Vergniory MG, Menshchikova TV, Silkin IV, Koroteev YM, Eremeev SV, Chulkov EV.

Physical Review B 92, 4 (2015)

150

Very large thermophase in ferromagnetic josephson junctions

Giazotto F, Heikkila TT, Bergeret FS.

Physical Review Letters 114, 067001 (2015)

151

Isotropically Polarized Speckle Patterns

Schmidt MK, Aizpurua J, Zambrana-Puyalto X, Vidal X, Molina-Terriza G, Saenz JJ.

Physical Review Letters 114, 113902 (2015)

152

Modifying the Interlayer Interaction in Layered Materials with an Intense IR Laser

Miyamoto Y, Zhang H, Miyazaki T, Rubio A.

Physical Review Letters 114, 116102 (2015)

153

Long-range spin accumulation from heat injection in mesoscopic superconductors with Zeeman splitting

Silaev M, Virtanen P, Bergeret FS, Heikkila TT.

Physical Review Letters 114, 167002 (2015)

154

Electronic Friction-Based Vibrational Lifetimes of Molecular Adsorbates: Beyond the Independent-Atom Approximation

Rittmeyer SP, Meyer J, Juaristi JI, Reuter K.

Physical Review Letters 115, 046102 (2015)

155

Time-Dependent Thermal Transport Theory

Biele R, D'Agosta R, Rubio A.

Physical Review Letters 115, 056801 (2015)

156

Optimized Effective Potential for Quantum Electrodynamical Time-Dependent Density Functional Theory

Pellegrini C, Flick J, Tokatly IV, Appel H, Rubio A.

Physical Review Letters 115, 093001 (2015)

157

Charge Redistribution and Transport in Molecular Contacts

Corso M, Ondracek M, Lotze C, Hapala P, Franke KJ, Jelinek P, Pascual JI.

Physical Review Letters 115, 136101 (2015)

158

Interplay of Surface and Dirac Plasmons in Topological Insulators: The Case of Bi_2Se_3

Politano A, Silkin VM, Nechaev IA, Vitiello MS, Viti L, Aliev ZS, Babanly MB, Chiarello G, Echenique PM, Chulkov EV.

Physical Review Letters 115, 21 (2015)

159

Exact Potential Driving the Electron Dynamics in Enhanced Ionization of H_2^+

Khosravi E, Abedi A, Maitra NT.

Physical Review Letters 115, 263002 (2015)

160

Depercolation of aggregates upon polymer grafting in simplified industrial nanocomposites studied with dielectric spectroscopy

Baeza GP, Oberdisse J, Alegria A, Saalwachter K, Couty M, Genix AC.

Polymer 73, 131 (2015)

161

Dielectric relaxations of Acrylic-Polyurethane hybrid materials

Martinez-Rugerio G, Alegria A, Daniloska V, Tomovska R, Paulis M, Colmenero J.

Polymer 74, 21 (2015)

162

Zwitterionic polymerization of glycidyl monomers to cyclic polyethers with $B(C_6F_5)_3$ (vol 5, pg 6905, 2014)

Asenjo-Sanz I, Veloso A, Miranda JI, Pomposo JA, Barroso-Bujans F.

Polymer Chemistry 6, 838 (2015)

163

Kohn-Sham approach to quantum electrodynamical density-functional theory: Exact time-dependent effective potentials in real space

Flick J, Ruggenthaler M, Appel H, Rubio A.

Proceedings of the National Academy of Sciences of the United States of America 112, 15285 (2015)

164

The nature of interfacial binding of imidazole and carbene ligands with M_{20} nanoclusters (M = Au, Ag and Cu) – a theoretical study

Geethalakshmi KR, Yang X, Sun Q, Ng TY, Wang D.

RSC Advances 5, 88625 (2015)

165

Determination of filler structure in silica-filled SBR compounds by means of saxs AFM

Otegui J, Miccio LA, Arbe A, Schwartz GA, Meyer M, Westermann S.

Rubber Chemistry and Technology 88, 690 (2015)

166

Active quantum plasmonics

Marinica DC, Zapata M, Nordlander P, Kazansky AM, Echenique P, Aizpurua J, Borisov AG.

Science Advances 1, e1501095 (2015)

167

New generation of two-dimensional spintronic systems realized by coupling of Rashba and Dirac fermions

Eremeev SV, Tsirkin SS, Nechaev IA, Echenique PM, Chulkov EV.

Scientific Reports 5, 12819 (2015)

168

Tunneling spectroscopy of close-spaced dangling-bond pairs in Si(001):H

Engelund M, Zuzak R, Godlewski S, Kolmer M, Frederiksen T, Garcia-Lekue A, Sanchez-Portal D, Szymonski M.

Scientific Reports 5, 14496 (2015)

169

Atomically precise semiconductor-graphene and *h*BN interfaces by Ge intercalation

Verbitskiy NI, Fedorov AV, Profeta G, Stroppa A, Petaccia L, Senkovskiy B, Nefedov A, Woll C, Usachov DY, Vyalikh DV, Yashina LV, Eliseev AA, Pichler T, Gruneis A.

Scientific Reports 5, 17700 (2015)

170

Universal Properties of Materials with the Dirac Dispersion Relation of Low-Energy Excitations

Protogenov AP, Chulkov EV.

Semiconductors 49, 1550 (2015)

171

Removal probability function for Kinetic Monte Carlo simulations of anisotropic etching of silicon in alkaline etchants containing additives

Zhang H, Xing Y, Gosalvez MA, Pal P, Sato K.

Sensors And Actuatuors A-Physical 233, 451 (2015)

172

Simulation guided design of globular single-chain nanoparticles by tuning the solvent quality

Lo Verso F, Pomposo JA, Colmenero J, Moreno AJ.

Soft Matter 11, 1369 (2015)

173

The universal trend of the non-exponential Rouse mode relaxation in polymer systems: a theoretical interpretation based on a generalized Langevin equation

Colmenero, J.

Soft Matter 11, 5614 (2015)

› Book chapters

- **Effect of Confinement Geometry on Out-of-Equilibrium Glassy Dynamics**
  D. Cangialosi
  Non-equilibrium Phenomena in Confined Soft Matter; Part of the series Soft and Biological Matter pp 265-298; ISBN: 978-3-319-21947-9 (2015)

- **Nanoparticles, Single-Chain: Nanomedicine**
  J. A. Pomposo
  Encyclopedia of Biomedical Polymers and Polymeric Biomaterials; ISBN: 978-1-43989-879-6 (2015)

- **Polymers: Single-Chain Polymer Nanoparticles**
  J. A. Pomposo
  CRC Concise Encyclopedia of Nanotechnology; ISBN: 978-1-46658-034-3 (2015)

Conferences

CFM-MPC scientists have organized or coorganized several international workshops and conferences during 2015. Many of these meetings have been held in close cooperation with Donostia Intenational Physics Center (DIPC), which shows the excellent results brought by the synergistic collaboration between both institutions.

The list of workshops organised by CFM-MPC researchers during 2015 follows:

- **Workshop MANA - DIPC. "Nanostructures and Complex Functional Materials"**
  August 27-28, 2015. Donostia International Physics Center, Donostia - San Sebastián. *Organisers:* Yutaka Wakayama (MANA, Japan) and Enrique Ortega (CFM-MPC).

- **Summer School "Frontiers of Condensed Matter 2015"**
  August 31 – September 11, 2015. Les Houches (France). *Organisers:* S. Bergeret (CFM-MPC), F. Hekking (Grenoble), J. Meyer (Grenoble) and J. van Ruitenbeek (Leiden).

- **The Ψ_k 2015 Conference**
  September 6-10, 2015. Kursaal Congress Centre, Donostia - San Sebastian. *Organisers:* Angel Rubio (CFM-MPC) and Risto Nieminen (University of Tech. Finland).

- **JCNS Workshop 2015: Neutron Scattering on Nano-Structured Soft Matter: Synthetic- and Bio-Materials**
  October 5-8, 2015. Tutzing, Germany. *Organisers:* Dieter Richter (Aachen, Germany) and Juan Colmenero (CFM-MPC).

- **21st International Workshop on Inelastic Ion-Surface Collisions (IISC-21)**
  October 18-23, 2015. Donostia-San Sebastián, Spain: *Organiser:* Iñaki Juaristi (CFM-MPC).

- **4th Baskrete Open Days to Industry**
  November 23-24, 2015, Donostia-San Sebastián. *Organisers:* Donostia International Physics Center, CEI Euskampus - EHU/UPV - Tecnalia - CFM/MPC.

- **Euskampus-Bordeaux SYMPOSIUM**
  November 26-27, 2015. Donostia - San Sebastián. *Organisers:* University of Bordeaux and Euskampus Aggregation, University of the Basque Country, Tecnalia, the Donostia International Physics Center, and CFM-MPC.

- **The 15th International Conference on Vibrations at Surfaces (VAS15)**
  June 22-26, 2015. Miramar Palace, Donostia - San Sebastián. *Organisers:* Andres Arnau (CFM-MPC), Giorgio Benedek, Eugene Chulkov (CFM-MPC), Asier Eiguren, Aran Garcia Lekue, Aitor Mugarza, Jose Ignacio Pascual and Thomas Frederiksen.

- **Workshop on "Theory for Planar Molecular and Atomic Scale Devices"**
  January 26-28, 2015. Donostia International Physics Center, Donostia - San Sebastián. *Organisers:* Daniel Sánchez-Portal (CFM-MPC), Mads Engelund (CFM-MPC), Thomas Frederiksen and Aran García-Lekue.

Research Funding

The following research projects are being developed at CFM-MPC during 2015. They cover a large variety of topics spred along the four research lines of the center. The projects running during 2015 are listed below according to the source of competitive funding, for every principal investigator (PI):

Projects funded by the Basque Government:

IT-578-13
Grupos consolidados: Simulación de sistemas cuánticos nanostructurados fuera del equilibrio
PI: Rubio Secades, Ángel

IT-621-13
Grupos de Investigación Consolidados y de Alto Rendimiento: Laboratorio de Nanofísica
PI: Ortega Conejero, Enrique

IT-627-13
Grupo de Investigación Consolidados
PI: Vitali, Lucia

IT-654-13
Polimeros y materiales no-cristalinos
PI: Colmenero de León, Juan

IT659-13
Grupo de Investigación Consolidado
PI: Balda de la Cruz, Rolindes

IT-756-13
Grupos de Investigación Consolidados y De Alto Rendimiento
PI: Arnau Pino, Andrés

IE14-393
NANOGUNE'14
BERC

Projects funded by the Spanish Ministry Science and Education:

FIS2011-27968
Estudio comparativo de la dinámica espectral y temporal de láseres
PI: Férnandez Rodríguez, Joaquín

FIS2013-41184-P
Optoelectrónica de gaps (sub)nanométricos plasmónicos para el desarrollo de espectroscopías y microscopías aumentadas de campo.
PI: Aizpurua Iriazabal, Javier

FIS2013-43130-P
Dynamical exchange-correlation effects in electronic and thermal transport
PI: Rubio Secades, Ángel

FIS2013-46159-C3-1-P
FUN-EMAT: Desarrollos fundamentales para la simulación y caracterización de procesos dinámicos fuera del equilibrio
PI: Rubio Secades, Ángel

FIS2013-48286-C2-1-P
Electronic processes in surfaces and nanostructures
PI: Ayuela Fernández, Andrés

FIS-2013-48286-C2-2-P
Reactividad, propiedades electrónicas y estructurales de sistemas complejos
PI: Juaristi Oliden, Iñaki

FIS2014-55987-P
Transporte de espin en estructuras híbridas: metales, superconductores, semiconductores, grafeno y aislantes topológicos
PI: Bergeret Sbarbaro, Sebastian

FIS2014-59264-REDC
Red Española sobre Ciencia, Aplicaciones y Tecnología de los Láseres Ultrarrápidos (CATLUR)
PI: Balda de la Cruz, Rolindes

MAT2012-31088
Estructura y dinámica de materiales complejos basados en polímeros
PI: Colmenero de León, Juan

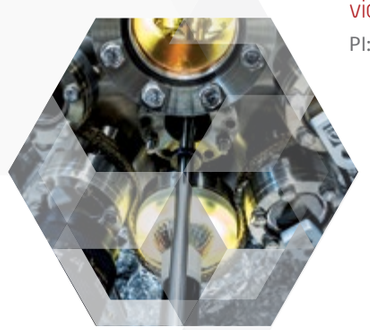
MAT2012-33720
Efectos magnetoeléctricos estáticos y ópticos en cristales
PI: Souza, Ivo

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

MAT2013-46593-C6-4P
Híbridos covalentes en superficies
PI: Ortega Conejero, Enrique

MAT2013-46593-C6-4P
Híbridos covalentes en superficies
PI: Vitali, Lucia

MAT2013-48246-C2-2-P
Efecto del procesamiento sobre las propiedades ópticas de vidrios y vitrocerámicos con aplicaciones fotónicas
PI: Balda de la Cruz, Rolindes



FIS2015-62538-ERC
Estrategias para el cosechamiento de la energía en la nanoescala
PI: Corso, Martina

CSD2010-00044:
Consolider nanoTHERM. Tailoring electronic and phononic properties of nanomaterials: Towards ideal Thermoelectricity
PI: Rubio Secades, Ángel

Proyect funded by CSIC

ICOOPLIGHT2015
Plasmónica Cuántica Activa en nanoantenas metálicas
PI: Aizpurua Iriazabal, Javier

Projects funded by the programs of the European Union:

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

FP7-ICT-2013-10 610446
PAMS: Plasmar Atomic and Molecular Scale devices
PI: Sánchez Portal, Daniel

7PM – People- CIG13/02
Magnetoelectric couplings in solids and releated phenomena
PI: Souza, Ivo

SEP-210187476
MOSTOPHOS: Modelling stability of organic phosphorescent light-emitting diodes
PI: Rubio Secades, Ángel

654360 - NFFA-Europe – RIA
Nanoscience foundries and fine analysis for Europe
PI: Rubio Secades, Ángel

FLAG-ERA-Trans2DTMD
Theoretical investigation of electronic transport in functionalized 2D transition metal dichalcogenides
PI: Rubio Secades, Ángel

MPNS COST Action MP12014
TERA-MIR Radiation: Materials, Generation, Detection and Applications
PI: Aizpurua Iriazabal, Javier

MPNS COST Action MP1401
Advanced fibre laser and coherent source as tools for society, manufacturing and life science.
PI: Fernández Rodriguéz, Joaquín

MPNS COST Action MP1403
Nanoscale Quantum Optics.
PI: Aizpurua Iriazabal, Javier

Other sources of International Funding

FA2386-15-1-0006 AOARD 144088
2D Materials and Devices beyond Graphene Science & Emerging Technology of 2D Atomic Layered Materials and Devices, US Air Force
PI: Rubio Secades, Ángel

Training

The Materials Physics Center (CFM-MPC) is a joint institute that depends on 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, trasnfering many of the values of the university-research center collaboration to the classroom. The standard higher education followed by a young student at CFM is associated to two degrees awarded by the corresponding associated departments at UPV/EHU:

- **Master in Nanoscience.** This is an official master program of UPV/EHU (held at CFM headquarters) and coorganized by the 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, development of topics related to nanomaterials and their applications, and a general knowledge on the research activity at the international level in the field of Nanoscience.

  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.

- **Physics of Nanostructures and Advanced Materials PhD program.** 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 (usually the Master's in Nanoscience program, although other similar degrees are accepted as well), 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 training on an individual basis. The list of PhD thesis works successfully defended at CFM in 2015 follows:

PhD Theses

Curved crystal surfaces: fabrication, characterization and growth of cobalt nanostructures
Student: Ana Magaña
Supervisor: Enrique Ortega
UPV/EHU

The role of H-bonds on the structure and dynamics of very concentrated polymer solutions
Student: Guido Goracci
Supervisors: Arantxa Arbe and Angel Alegria
UPV/EHU

Spectroscopic analysis of atoms and molecules
Student: Alison Crawford Uranga
Supervisors: Stefan Kurth and Angel Rubio
UPV/EHU

On the dielectric properties of water confined in cement-like materials
Student: Manuel Monasterio Jaqueti
Supervisor: Silvina Cerveny Murcia
UPV/EHU

Theory and simulation of the optical response of novel nanomaterials from visible to terahertz
Student: Mohamed Ameen Poyli
Supervisors: Rubén Esteban and Javier Aizpurua
UPV/EHU

Density-Potential Mapping in the Standard and Quantum Electrodynamical Time-Dependent Density Functional Theory
Student: Mehdi Farzanehpour
Supervisors: Ilya Tokatly and Angel Rubio
UPV/EHU

Optimisation of the first principle code Octopus for massive parallel architectures: application to light harvesting complexes
Student: Joseba Alberdi-Rodriguez
Supervisors: Javier Muguerza and Angel Rubio
UPV/EHU

Master Theses

Synthesis and relaxation dynamics of cyclic polyethers
Student: Thomas Gambino
Supervisor: Fabienne Barroso-Bujans
UPV/EHU

Zwitterionic Ring Opening Polymerization for theConstruction of Complex Nano-objects
Student: Jon Rubio Cervilla
Supervisors: José A. Pomposo and Fabienne Barroso-Bujans
UPV/EHU

New photoactivated routes to bioinspired single-chain polymer nanoparticles
Student: Sajad Jalilian
Supervisor: José A. Pomposo
UPV/EHU

Investigation of the structure of curved single crystal surfaces of Pd and Ni
Student: Erika Alexandra Montero Lebron
Supervisors: Enrique Ortega and Maxim Ilin
UPV/EHU

SYNTHESIS OF CYCLIC POLYETHERS
Student: Dannia Esther Guzman Pimentel
Supervisor: Fabienne Barroso-Bujans
UPV/EHU

STM and LEED characterization of F4TCNQ molecules self-assembly on BiAg2/Ag(111) surface alloy
Student: Néstor Merino Díez
Supervisors: Dimas García de Oteyza and Guillaume Vasseur
UPV/EHU

Undergraduate Courses

In addition to the Master's and PhD programs, the staff at CFM-MPC 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-MPC staff.

PhD students seminars

Since 2013, a regular series of seminars delivered by PhD students is organized at CFM. This activity continued during 2015. 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, this activity helps to improve the internal communication about the research activity going on in the center.

Internship

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

CFM-MPC provided two summer internships to undergraduate students during 2015:

- Mikel Andonegui Isasa working at the Polymers and soft Matter research line with J. Pomposo
- Ruben Tejero Bonacasa working at the Polymers and soft matter research line with A. Arbe

Outreach

CFM-MPC is developing a broad program of activities aimed at bringing the excitement of science to young people. Among these activities, particular effort is devoted to secondary-level and high-school students, with an overall goal of increasing student and teacher enthusiasm for scientific research. Since September 2013, every two weeks, several schools have visited CFM facilities, sharing these efforts in joint activities with DIPC.

The list of schools visiting the CFM laboratories during 2015 follows:

School	Date	Number of students	Group
2014-2015 course			
IES Urola	26/02/2015	28	2nd course high school
Summa Aldapeta Ikastetxea	13/03/2015	44	2nd course high school
Usandizaga Institutoa	26/03/2015	51	2nd course high school
Irungo Pio Baroja Institutoa	17/04/2015	45	2nd course high school
URRETXU-ZUMARRAGA IKASTOLA	24/04/2015	35	2nd course high school
Axular Lizeoa	08/05/2015	15	2nd course high school
2015-2016 course			
La Anunciata de San Sebastián	03/10/2015	22	1st - 2nd course high school
Laskorain ikastola	16/10/2015	27	2nd course high school
BHI Beasain	30/10/2015	35	2nd course high school
Manteo- Zubiri Institutoa	20/11/2015	43	2nd course high school
Larramendi ikastetxea	27/11/2015	22	2nd course high school
J.M.Iparragirre B.H.I. Urretxu	17/12/2015	14	2nd course high school
	TOTAL	381	

› Others outreach activities

Researchers at CFM-MPC are fully commited to spread the activities in the center to society at many different levels. Some of the activities where CFM-MPC staff participated during 2015 follows:

- **Imaginenano 2015**
  March 10-13, 2015. Bilbao - Phantoms Foundation, CIC nanoGUNE, DIPC and CFM. Stand showing the research activity at CFM-MPC coordinated by CFM-MPC project manager Francisco López Gejo, in coordination with DIPC and nanoGUNE.

- **Mestizajes**
  A través del espejo: La literatura mira a las científicas.
  Abril 28, 2015. Donostia. Museo San Telmo (STM) - DIPC - CFM-MPC. Talks and debates about the mixing of Science and Literature directed by CFM-MPC researcher Gustavo Schwartz.

- **San Sebastian Software Carpentry Workshop 2015**
  June 15-16, 2015, Donostia. Materials Physics Center - University of the Basque Country. Workshop on software skills given by CFM IT manager Iñigo Aldazabal to a community of IT programmers.

- **Pint of Science**
  June 18, 2015, Ni Neu Bar in San Sebastián, Outreach talk to the general public “La luz en la Nanoescala” by CFM-MPC researcher Javier Aizpurua, simultaneously with many other scientific talks in bars all over different cities in Europe.

- **Semana de la Ciencia**
  Noviembre 5-7, 2015 Donostia. Set of activities at Museo San Telmo plaza Zuloaga, devoted to promote scientific culture among primary school students. This action is coordinated by researcher Celia Rogero at CFM, in collaboration with researchers at DIPC and nanoGUNE.

Transfer of Knowledge

CFM-MPC is constantly seeking to maximize the impact of the scientific activity developed in the center with the aim to provide return to our society, therefore any opportunity for transferring knowledge is conveniently exploited through a careful analisis of technical potentials found in the center as well as a market prospective.

Cooperation with industry at CFM-MPC is channeled through two different paths: Collaborative Research and Technical Services. Both forms of cooperation are backed up by the experienced Technology Transfer Offices and Administrative Services from CSIC and UPV/EHU.

In collaborative research, CFM teams up with industrial actors, and often with other research institutions, for addressing complex technological challenges. Projects typically aim at innovative technological solutions which provide a competitive edge and have direct impact in the commercial activity of the industrial partners. Thanks to the high-profile and excellence in research activity, CFM-MPC scores high in competitive calls, which provide financial support for these activities. Through technical services, CFM allows industrial actors to have access to its singular, state-of-the-art infrastructure and the experience and skills of its staff. Services can be hired at convenience and scaled to fit the needs, from single measurements to regular, recurrent analysis. Since 2015 a chart of services has been designed at CFM-MPC together with the central CSIC services as well as with the Basque Office of Innovation, Innobasque.

CFM is committed to close the gap between Fundamental Research and Industrial activity. This is important not only for transferring knowledge but also for providing professional opportunities for our highly-skilled students and young researchers. Spin-off projects are important tools for this, as they provide our entrepreneurs to develop technological enterprises based in our know-how and technologies.

Currently, there are three on-going projects connected with transfer of knowledge:

- BIHURCRYSTAL (www.bihurcrystal.com), the first and most developed project so far, provides technology for ultra-high vacuum environments (scientific infrastructure and space applications). After winning Manuel Laborde and Toribio Echeberria Prizes in 2012 and 2013, respectively, as entrepreneurial project, the company constituted in 2013 and commercializes its first products, based in technologies developed at CFM and the CAB (Centro de Astrobiología, Madrid). BIHURCRYSTAL has attracted investment from SPRI CAPITAL RIESGO and important competitive funding such as from programs such as RETOS COLABORACION and NEOTEC. As of 2015, the company employs four Doctors and one technician, all former students of CFM and ICMM (Instituto Ciencia Materiales Madrid).

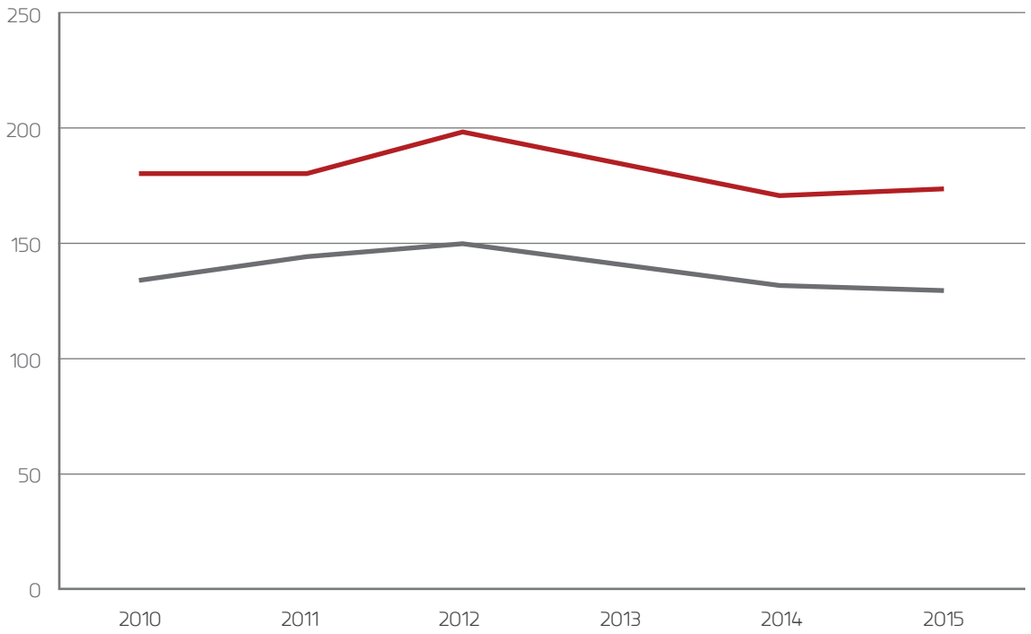
- MATERIALS EVOLUTION (http://www.etsf.eu/materials_evolution) focuses in applying theoretical modelling and simulation methods for accelerating the development of new materials. The initiative at CFM-MPC is supported by the European Theoretical Spectroscopy Facility, and runs in parallel with counterparts in Sweden and Belgium, aiming to provide a service with coverage over the whole European Region. MATERIALS EVOLUTION has received the Manuel Laborde Prize in 2015.

- BASKRETE ENERGY, the youngest project, 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.

CFM gratefully acknowledges support by BIC BERRILAN in the development of all these projects that continue being developed during 2015.

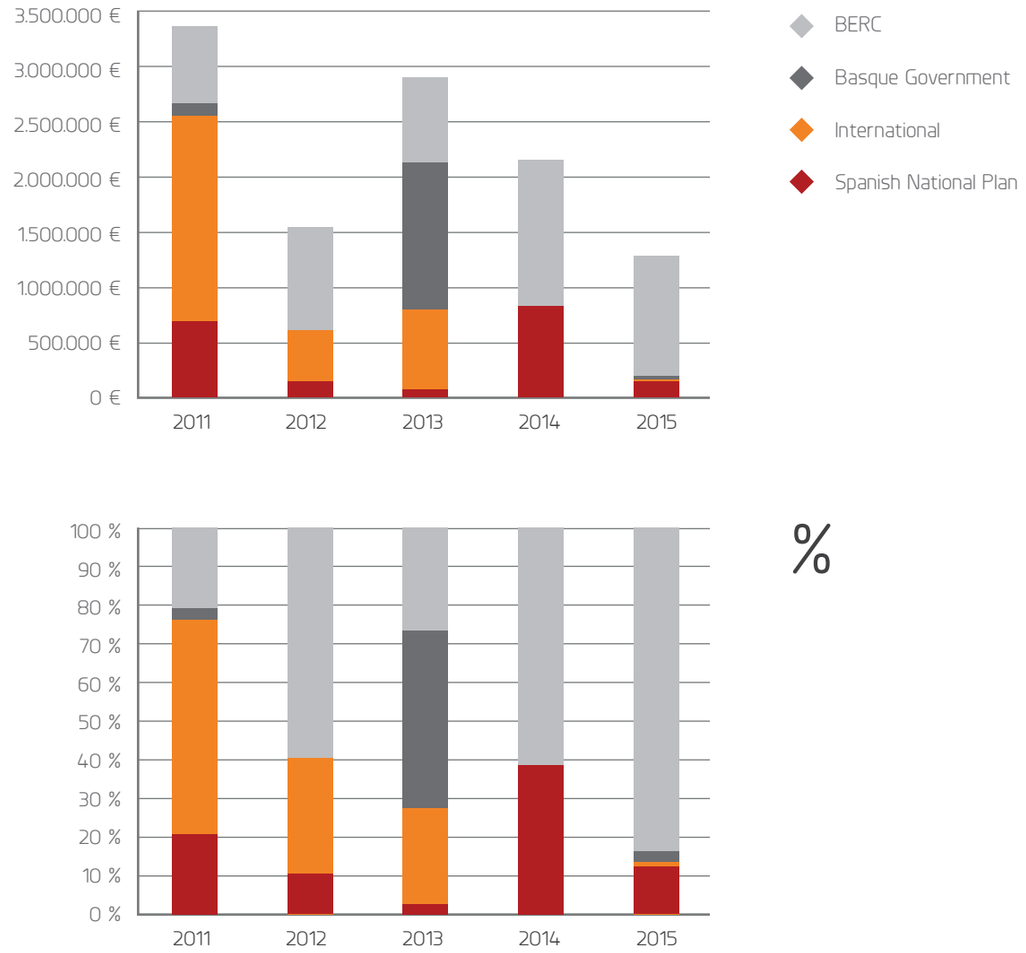
Appendix

› Publications 2010-2015



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

› Projects CFM 2010-2015



	Spanish National Plan	International	Basque Government	BERC
2011	691.514,00 €	156.500,00 €	105.000,00 €	691.514,00 €
2012	156.090,00 €	469.895,62 €	0,00 €	918.757,39 €
2013	76.050,00 €	719.996,00 €	1.350.695,00 €	768.908,68 €
2014	838431,23 €	0,00 €	0,00 €	1.316.778,45 €
2015	156.500,00 €	15.600,00 €	34.668,00 €	1.073426,00 €

Human Resources CFM 2010-2015

%

	2010	2011	2012	2013	2014	2015
CSIC	49	49	39	30	25	25
UPV-EHU	36	35	37	35	40	36
BERC	4	4	10	17	25	29
IKERBASQUE	2	5	7	6	7	8
Colaborators	0	2	5	5	5	5
	91	95	98	93	102	103

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