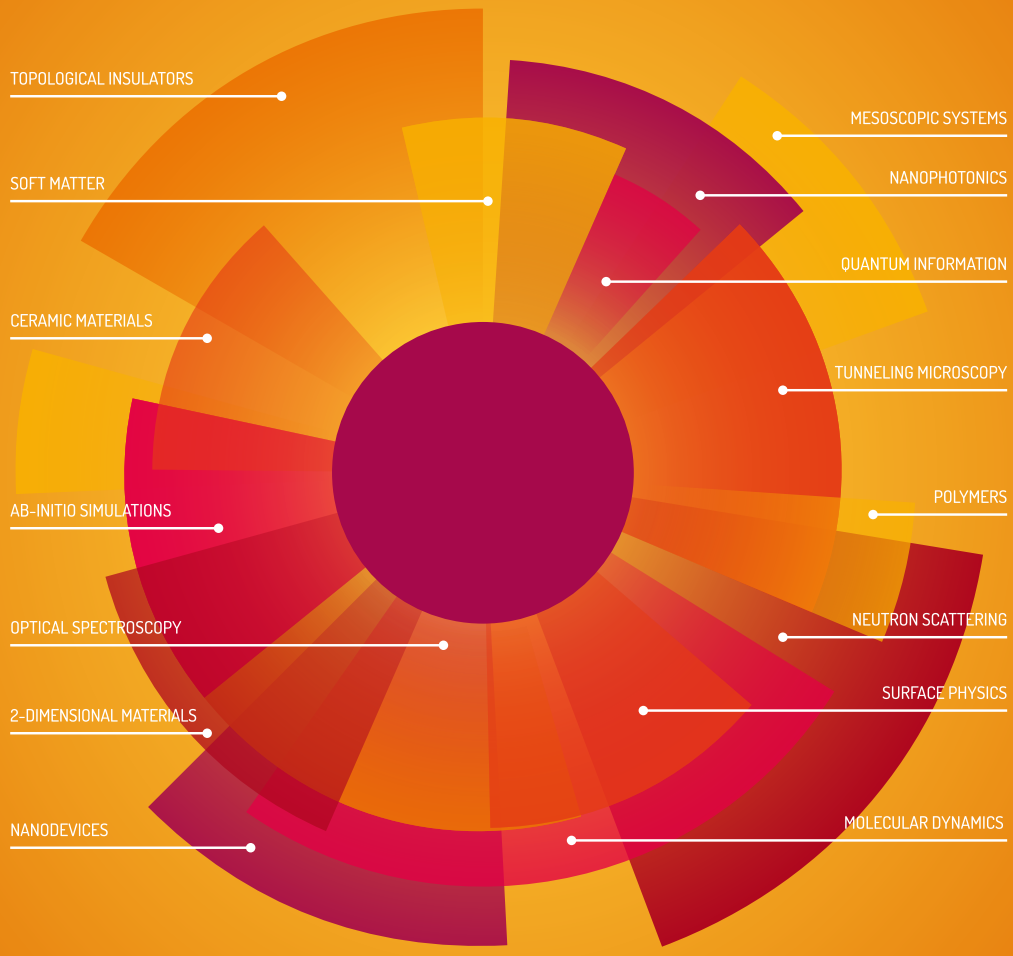
ACTIVITY REPORT

Centro de Física de Materiales
Materialen Fisika Zentroa
Materials Physics Center

CFM



2017

CSIC
Consejo Superior de Investigaciones Científicas

eman ta zabal zazu
Universidad del País Vasco
Euskal Herriko Unibertsitatea

MPC-BERC
Materials Physics Center
Basic Excellence Research Centre

ACTIVITY REPORT 2017

CFM

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SUMMARY

SUMMARY

FOREWORD

Andrés Arnau Pino, Vice-Director

"A centre can only be excellent if it is excellent in all senses"

2017 has been an important year at the Center for Materials Physics CFM-MPC. First of all, two new scientists joined the scientific board as permanent members of the Centre. Martina Corso was formally appointed tenured scientist of the Spanish Council for Scientific Research (CSIC), and Gabriel Molina Terriza joined as an Ikerbasque Professor associated to the Materials Physics Center (MPC). Martina is joining the Nanophysics Laboratory group, and Gabriel takes the responsibility of launching a new experimental laboratory of Quantum Nanooptics. Our permanent team of scientists has thus increased by two new members who are warmly welcomed to our centre. After these recruitments, the number of groups in the Centre is set up to 15, covering a diverse variety of fields in different disciplines of Materials Science.

Secondly, the External Advisory Board visited our centre for the first time and performed a thorough analysis of the Centre's capabilities, its strategic plan, and its potential for future development, which also consisted of individual interviews with each of the groups. It was amazing to witness how every group in the Centre reacted to this visit by collecting and preparing a very complete set of reports on the performance, the strategy and the self-analysis of their respective scientific activities. This piece of information was relevant not only for the evaluation by the External Advisory Committee, but also to launch other important strategic actions in the Centre as we will detail below. We would like to truly thank all the groups for their quick and complete analysis of their activities and the timely filing of the reports. This was absolutely instrumental to make strategic decisions in the Centre.

Following the valuable information collected by the groups, the strategic plan of the Centre for 2018-2021 was conceived and developed during the first months of 2017. Different aspects of the Centre's plan were added to the strategic plan of the Area of Materials at CSIC, which was also added to the overall generic CSIC strategic plan for 2018-2021.

The University of the Basque Country (UPV/EHU) and the Spanish Council for Scientific Research (CSIC) are the two key institutions which govern and support the Center for Materials Physics (CFM). Both of them have been ruling our joint-centre with clear vision and commitment. A new direction board at UPV/EHU has taken over during 2017 which, together with the direction board at CSIC, has continued the long-standing support to CFM. We are proud to say that the collaboration between UPV/EHU and CSIC at the Center for Materials Physics in Donostia-San Sebastián is a good example of synergy between two respected institutions that provide an added value to the scientific activity of excellence in a centre.

Javier Aizpurua Iriazabal, Director

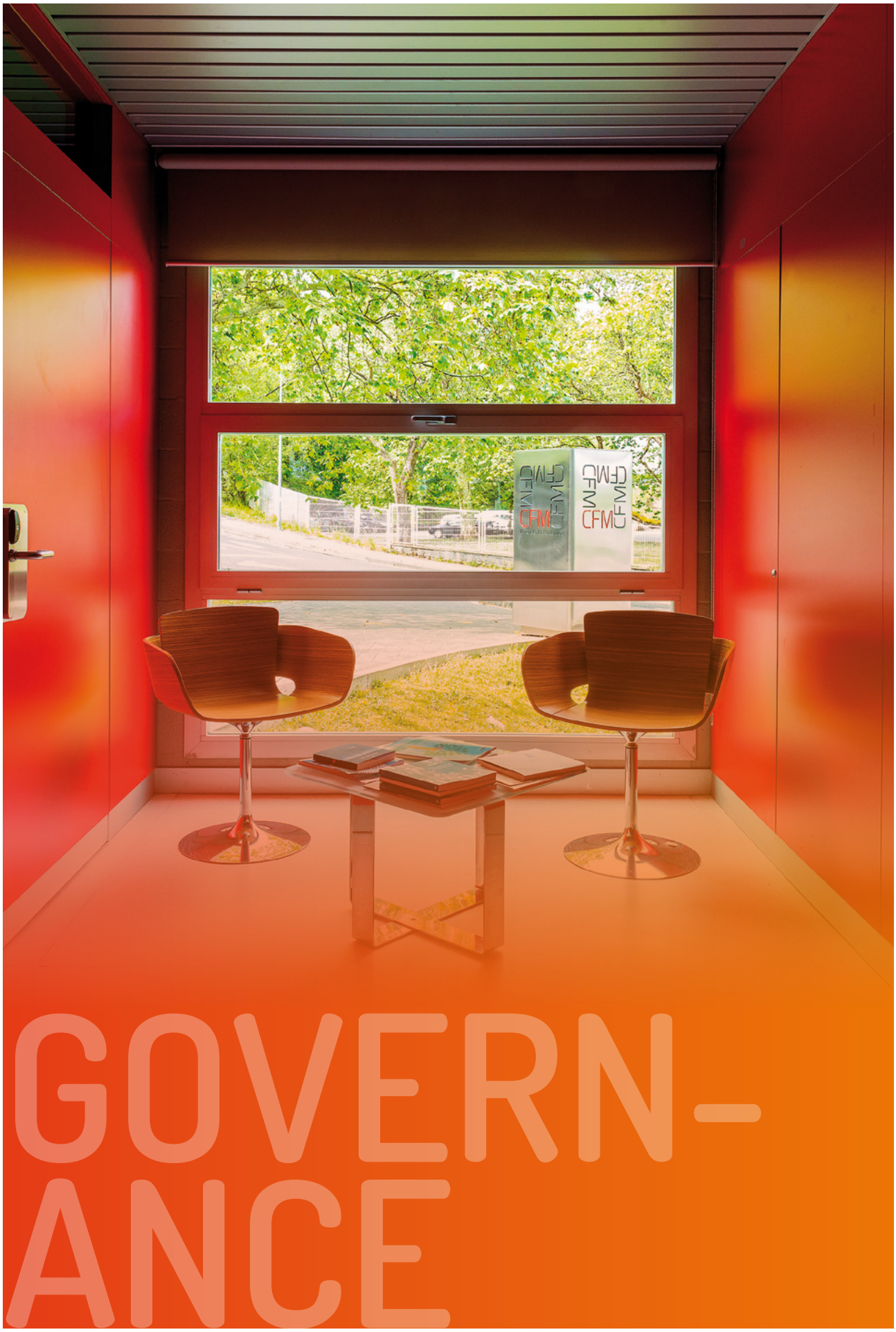
"The human team at CFM-MPC continues being the most important asset we have"

A third key partner in our centre is the Basque Government. The Department of Education, Research and Universities, along with Ikerbasque, has supported enormously the activity of our centre through the "Basic Excellence Research Center" (BERC) program. CFM has been declared a BERC by the Basque Government during the last years, providing a qualitative and quantitative step forward in resources to the Centre. 2017 has been the last year of the BERC 2014-2017 program, and a new call for 2018-2021 was opened during 2017. The input provided by the scientific groups at the Centre, together with the huge effort by the administrative staff, has allowed the preparation of a successful proposal for 2018-2021, which has just been approved and accepted by the Basque Government. The commitment and dedication found in our administration staff has exceeded all the expectations. A centre can only be excellent if it is excellent in all senses. We can proudly state that the administration staff is as excellent as the scientific staff, and this has been one of the key aspects of the success of the current BERC program. In this context, at the end of 2017, Amaya Moral, CFM administration manager, left the Centre to continue a different professional path. Amaya has been an inspiring driving force of the CFM-MPC administration during the last years. We thank all her work and professionalism and wish her all the best in the new stage.

Finally, the Gipuzkoa Foru Aldundia, Gipuzkoa's Province Government, has also supported several activities in the Centre through different research and innovation programs, and proudly takes part in the Board of MPC. We are also grateful for this.

With the security that provides the strong commitment of our institutions, we can safely trust in an excellent development of our centre for the coming years. As you will check in this "Report of Activities", 2017 has been a very good year in all senses at CFM: our scientific output has been excellent, we have deeply improved the success in European calls, we maintain our high international profile very active, we have implemented a self-assessment of our reality to keep improving, we have increased the quantity and quality of new cohorts of PhDs, we have reached better to our society and enhanced our visibility, we have secured the future of key activities in the Centre during 2018-2021 through the BERC program, and more importantly, we are building a community of people who feel proud of belonging to CFM-MPC. The human team at CFM-MPC continues being the most important asset we have. Thank you all for your commitment, dedication, and constructive attitude towards a better centre.

Warm greetings,
Javier Aizpurua and Andrés Arnau



GOVERN-ANCE

GOVERNANCE

Centro de Física de Materiales (CFM) is a joint centre 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 Centre 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 Centre. To that end the Direction board is supported by the Centre's Board and the Scientific Board.

The Association "Materials Physics Center" MPC is a non-profit association declared as Basic 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 appoints 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.

CFM

CSIC

UPV/EHU

Chemical Physics of Complex Materials

Electronic Properties at the Nanoscale

Photonics

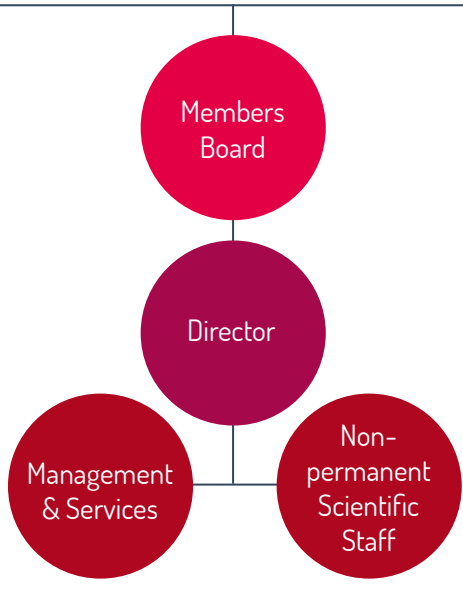
Polymers and Soft Matter

MPC - BERC

DIPC

GV

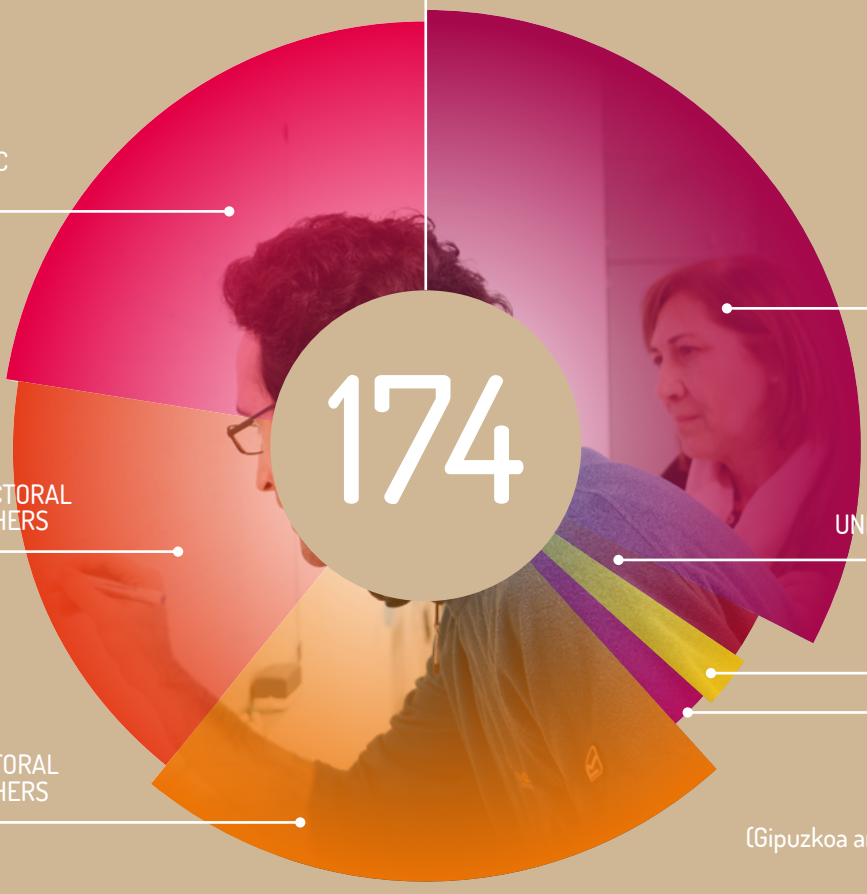
Diputación de Gipuzkoa



PROFILE

SCIENTIFIC COMMUNITY

Researchers in action



39 SCIENTIFIC SENIOR

29 POST-DOCTORAL RESEARCHERS

39 PRE-DOCTORAL RESEARCHERS

57 VISITORS

3 UNDERGRADUATE INTERNSHIPS

4 TECHNICIANS

3 FELLOWS (Gipuzkoa and Ikerbasque)

Research groups
15

Researchers from
21
countries

49%
of the research community is international

TRAINING

PhD Theses defended
12

Master Theses defended
9

RESEARCH OUTPUT

ISI Publications
183

Average impact factor
5.90

H-index
109

Q1 Publications
116

Citations*
10 240

*Source Web of Science Core Collection- CFM's Researcher ID: F-4867-2012 as of March 2018

ACTIVITIES AND EVENTS

Seminars
15

Workshops and conferences
12

Visitors from high schools
424

Outreach activities
9

Impact in the media
129

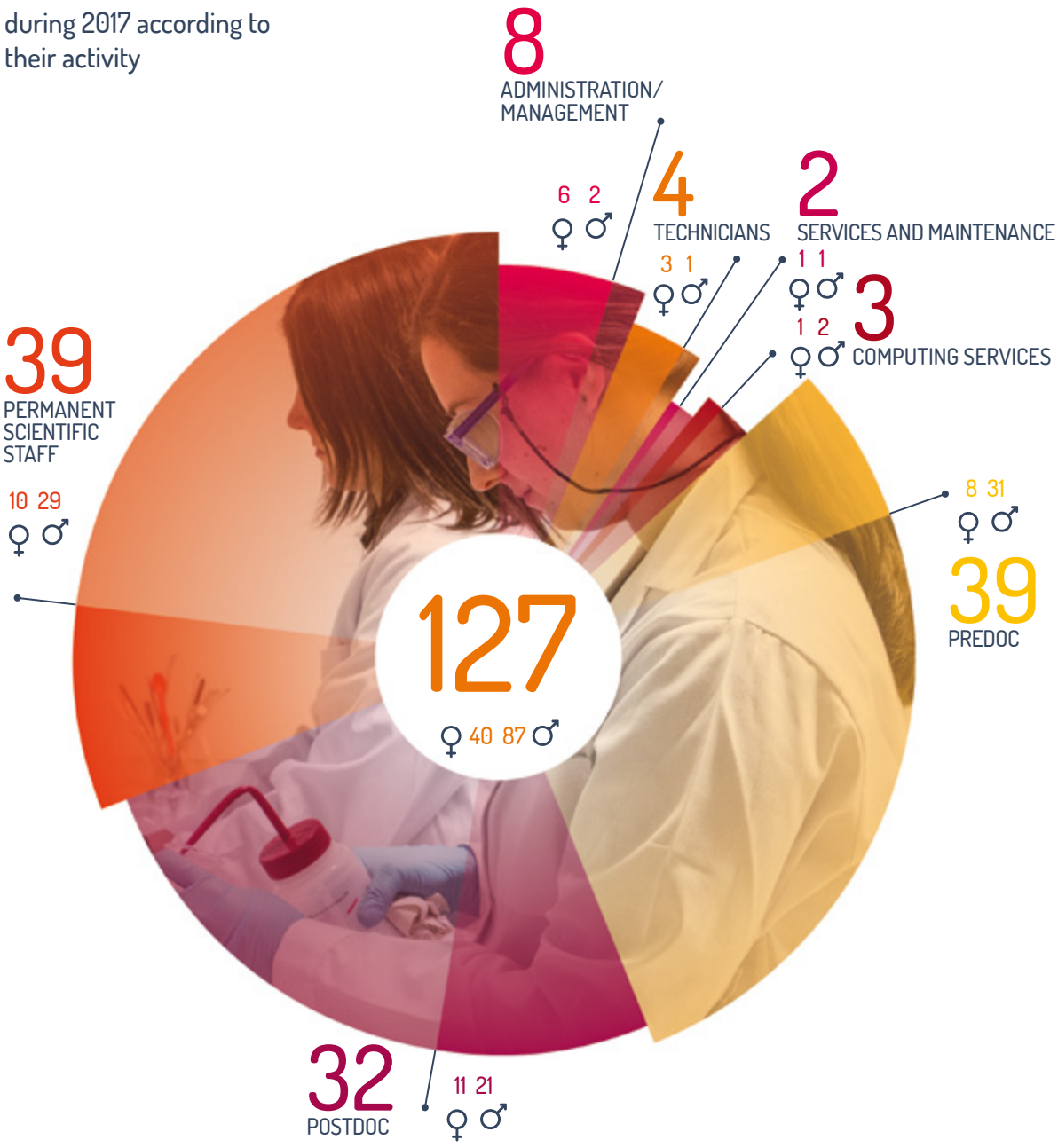
PROJECTS AND FUNDING

Ongoing projects
49

Funding 2017
2 444 817€

PEOPLE

Distribution of CFM staff during 2017 according to their activity

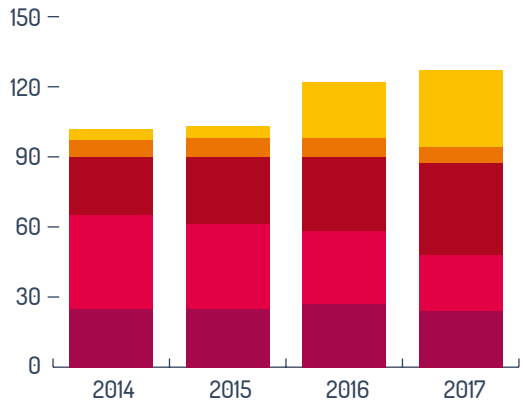


PEOPLE AT A GLANCE

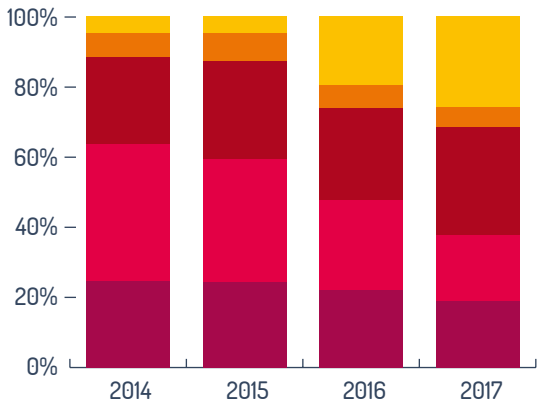
	2014	2015	2016	**2017**
CSIC	25	25	27	**24**
UPV	40	36	31	**24**
MPC-BERC	25	29	32	**39**
IKERBASQUE	7	8	8	**7**
COLLABORATORS*	5	5	24*	**33**
Total	102	103	122	**127**

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

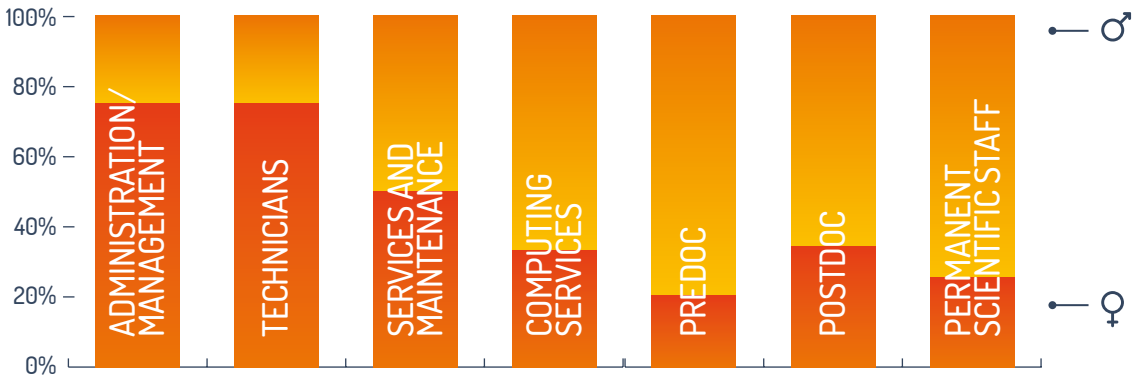
Distribution of staff at CFM in absolute numbers according to their origin through the last years.



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



Staff distribution at MPC-CFM according to category and gender.



DIRECTION BOARD

Javier Aizpurua Iriazabal, Director

Andrés Arnau Pino, Vicedirector

Amaya Moral Arce, General Manager

MANAGEMENT

Amaya Moral Arce, Administration Manager, CSIC

María Formoso Ferreiro, Administrative, MPC

Ane Iturriza Semperena, Administrative, MPC

Txema Ramos Fernández, Administrative, CSIC

Jasone Ugarte García de Andoin, Executive Secretary, UPV/EHU

Francisco López Gejo, Project Manager, MPC

Elixabet Sarasketa Zabala, Project and Technology Transfer Manager, MPC

Idoia Mugica Mendiola, Outreach Manager, MPC

COMPUTING SERVICES

Iñigo Aldazabal Mensa, Computer Centre Manager, CSIC

Ioritz Paulis Garmendia, IT Systems Technician, MPC

Garbiñe Egaña Cruz, IT Systems Technician, MPC

Beñat Jimenez Urbieta, Undergraduate student

SERVICES AND MAINTENANCE

Tamara Molina Rolo, Services, MPC

Juan Manuel Burgos Jiménez, Maintenance, MPC

RESEARCHERS

Research Line:

Chemical Physics of Complex Materials

01 Gas/Solid Interfaces

Staff

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

Postdoctoral Researcher

Natalia Koval

Predoctoral Researchers

Ivor Lončaric
Alejandro Peña Torres

02 Souza Research Group

Staff

Ivo Souza, Ikerbasque Professor, UPV/EHU

Postdoctoral Researchers

Stepan Tsirkin
Julen Ibañez Azpiroz
Tomas Rauch

03 Nanophysics lab

Staff

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

Ikerbasque Fellow

Sara Barja Martínez, UPV/EHU

Postdoctoral Researchers

Marco Gobbi
Maxim Ilin
Jens Brede
Luciano Colazzo
Laura Fernández Gómez –Recuero
Zakaria Abd-El Fattah

Predoctoral Researchers

Ignacio Piquero Zulaica
Mikel Abadía Gutiérrez
Fernando García Martínez
Wen Wan

Undergraduate Students

Ander Arregui Biera
Irati Garmendia San Miguel
Anna Oelsch

04 Modelisation and Simulation

Staff

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

Postdoctoral Researchers

Mikhail Otrokov
Pedro Brandimarte Mendonça
Fernando Delgado Acosta
Predoctoral Researchers
Iker Gallardo Arrieta
Marc Barbry
Moritz Mueller

05 Spectroscopy at Atomic Scale

Staff

Lucia Vitali, Ikerbasque Professor, UPV/EHU

Predoctoral Researchers

Alexander Correa
Ana Barragán Duran

Research Line:

Electronic Properties at the Nanoscale

06 Electronic Excitations in Surfaces and Nanostructures

Staff

Andrés Ayuela Fernández, Scientific Researcher, CSIC

Pedro Miguel Echenique Landiribar, University Professor, UPV/EHU

Evgeni V. Tchoulkov, University Professor, UPV/EHU

Postdoctoral Researchers

Ilya Nechaev

Jhon Wilfer González Salazar

Marta Pelc

Romain Dupuis

Predoctoral Researchers

Tomás Alonso Lanza

Raul Guerrero Avilés

07 Materials Computation and Theory

Staff

Aitor Bergara Jauregi, Associated Professor, UPV/EHU

José María Pitarke de la Torre, University Professor, UPV/EHU

Predoctoral Researchers

Unai Aseguinolaza Aguirreche

Miguel Borinaga Treviño

Iñigo Robredo Magro

08 Mesoscopic Physics

Staff

F. Sebastián Bergeret Sbarbaro, Tenured Scientist, CSIC

Ikerbasque Fellow

Vitaly Golovach, UPV/EHU

Postdoctoral Researchers

Tineke Van Den Berg

Predoctoral Researchers

Alba Pascual Gil

Cristina Sanz Fernández

Mikel Rouco Martín

Xian-Peng Zhang

Undergraduate Student

Alberto Hijano Mendizabal

09 Nano-Bio Spectroscopy

Staff

Ángel Rubio Secades, University Professor, UPV/EHU

10 Quantum Phenomena on Surfaces

Staff

Nicolas Lorente Palacios, Scientific Researcher, CSIC

Predoctoral Researchers

José Reina Gálvez

Research Line:

Photonics

11 Theory of Nanophotonics

Staff

Javier Aizpurua Iriazabal, Research Professor, CSIC

Alberto Rivacoba Ochoa, University Professor, UPV/EHU

Nerea Zabala Unzalu, Associate Professor, UPV/EHU

Postdoctoral Researchers

Mario Zapata

Yao Zhang

Predoctoral Researchers

Garikoitz Aguirregabiria Achutegi

Andrea Koneçna

Tomas Neuman

Álvaro Nodar Villa

Mattin Urbieta Galarraga

Antton Babaze Aizpurua

12 Nanomaterials and Spectroscopy

Staff

Yury Rakovich, Ikerbasque Professor, UPV/EHU

Postdoctoral Researcher

Thomas Hendel

13 Laser Physics and Photonic Materials

Staff

Rolindes Balda de la Cruz, University Professor, UPV/EHU

Joaquín Fernández Rodríguez, Emeritus University Professor, UPV/EHU

14 Quantum Nanophotonics Laboratory

Staff

Gabriel Molina Terriza, Ikerbasque Professor, MPC

Research Line:

Polymers and Soft Matter

15 Polymers and Soft Matter

Staff

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

Postdoctoral Researchers

Ana Lucia Rodríguez Garraza
Edurne Gonzalez Gándara
Guido Goracci
Izaskun Letizia Combarro Palacios
Beatriz Robles Hernández
Daniel Enrique Martínez Tong
Paula Ángela Malo de Molina Hernández
Xavier Monnier

Predoctoral Researchers

Alejandro Latorre Sánchez
Jon Rubio Cervilla
Jorge Melillo
Julen De la Cuesta Leone
Lucia Ortega Álvarez
Marina González Burgos
Maud Formanek
Natalia Gutiérrez Pérez de Eulate
Thomas Louis Gambino
Jordan Ochs

Scientific Technicians

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

Undergraduate Students

Iker Castrillo Maestro
Usue Aspiazu Iturbe
Julen Gorospe Trujillo
Ane Puente Irizar
Maitane Romatet Larrañaga

OTHER POSITIONS

Staff

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

Professors

Miguel Ángel Cazalilla Gutierrez, CSIC
Fabian Barroso, Ikerbasque Research Professor, DIPC
Dimas García de Oteyza, Ikerbasque Research Professor, DIPC

Postdoctoral Researchers

Pawel Nita (Dimas Garcia de Oteyza´s group, DIPC)

Predoctoral Researchers

Nestor Merino Diez (Dimas Garcia de Oteyza´s group, DIPC)
Mohammed Sabri Gamal (Dimas Garcia de Oteyza´s group, DIPC)

Visitors

CFM received 57 visiting researchers during 2017.

EXTERNAL ADVISORY COMMITTEE

EXTERNAL ADVISORY COMMITTEE

Professor Peter Saalfrank

Institut für Chemie,
Universität Potsdam, Germany

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

- **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 Interests:** Theoretical Surface Science, System-bath quantum dynamics, Laser-driven electron dynamics, Theoretical photophysics and chemistry, Electronic structure theory
- **Publications:** More than 175 ISI papers
- Regular visitor of the DIPC and CFM.

Professor Antonio Hernando Grande

Universidad Complutense de Madrid, Spain

Director of "Instituto de Magnetismo Aplicado" (IMA)

- **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 Interests:** 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
- Regular visitor of the DIPC, the CFM and the UPV/EHU.

Professor Francisco J. García Vidal

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

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

- **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 Interests:** Photonics, Nanophotonics
- **Publications:** More than 280 ISI papers
- Regular visitor of the DIPC and CFM.

Professor Dr. Dieter Richter

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)

- **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 Interests:** Structure and Dynamics of Polymers and Soft Matter; Neutron Techniques and Instrumentation.
- **Publications & Patents:** More than 450 ISI papers
- Regular visitor of the DIPC and CFM.

RESEARCH LINES, GROUPS & HIGHLIGHTS

Within the general objective to target excellence in the research on materials physics, CFM has focused on four main strategic forms of matter that cover some of the main structures and systems in advanced materials research: (I) Molecules, (II) Solid State Systems, (III) Photonics, and (IV) Polymers. The research activities in the centre have thus been structured during the last years into the corresponding four research lines that give response to the aforementioned targets. The current research lines in the centre are: (i) CHEMICAL PHYSICS OF COMPLEX MATERIALS, (ii) ELECTRONIC PROPERTIES AT THE NANOSCALE, (iii) PHOTONICS and (iv) POLYMERS AND SOFT MATTER. Gathered under this four **Research lines**, at CFM the fundamental unit of organisation is the **Research Group**, although the structure remains fully horizontal, actively seeking cross-linked, multidisciplinary research. Until 2017, fourteen groups coexisted in the development of CFM research activity, each of them led by one permanent member of the scientific staff. During 2017, a new group has been created at CFM, led by Ikerbasque Professor Gabriel Molina Terriza. Prof. Molina Terriza has launched the "Quantum Nanophotonics Laboratory" group in June 2017, associated to the Research Line of Photonics. The Quantum Nanophotonics laboratory is being developed during 2018. With this new group, the total number of groups at CFM sums up to fifteen.

RESEARCH LINES, GROUPS AND HIGHLIGHTS

RESEARCH LINE	GROUP	PROFILE
Chemical Physics of Complex Materials	01 GAS/SOLID INTERFACES	Theoretical
	02 SOUZA RESEARCH GROUP	Theoretical
	03 NANOPHYSICS LAB	Experimental
	04 MODELISATION AND SIMULATION	Theoretical
	05 SPECTROSCOPY AT ATOMIC SCALE	Experimental
Electronic Properties at the Nanoscale	06 ELECTRONIC EXCITATIONS IN SURFACES AND NANOSTRUCTURES	Theoretical
	07 MATERIALS COMPUTATION AND THEORY	Theoretical
	08 MESOSCOPIC PHYSICS	Theoretical
	09 NANO-BIO SPECTROSCOPY	Theoretical
	10 QUANTUM PHENOMENA ON SURFACES	Theoretical
Photonics	11 THEORY OF NANOPHOTONICS	Theoretical
	12 NANOMATERIALS AND SPECTROSCOPY	Experimental
	13 LASER PHYSICS AND PHOTONIC MATERIALS	Experimental
	14 QUANTUM NANOPHOTONICS LABORATORY	Experimental
Polymers and Soft Matter	15 POLYMERS AND SOFT MATTER	Theoretical and Experimental

Twelve of the groups develop their activity in the premises of CFM in Donostia-San Sebastián, while the laboratories of the "Laser Physics and Photonics Materials" group are located at the Engineering School of Bilbao (UPV/EHU), the "Materials Computation and Theory" group develops its activity in the Science Faculty of Leioa, and the "Nano-Bio Spectroscopy" group is located in the Joxe Mari Korta research building (UPV/EHU), in the Ibaeta Campus in Donostia-San Sebastián.

CHEMICAL PHYSICS OF COMPLEX MATERIALS

The research line “Chemical Physics of Complex Materials” addresses the structural and electronic properties of complex nanostructured materials, particularly in the presence of molecules. Five research groups are included in this research line, with a high degree of complementarity. 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 Interfaces” group, the “Modelisation and Simulation” group, and the “Souza Research 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 are the “Nanophysics Laboratory” and the “Spectroscopy at Atomic Scale” groups.

In what follows, the strategic activity of the five research groups included in this research line is described.

01 Gas/Solid Interfaces

Group leader: Ricardo Díez Muiño, Scientific Researcher, CSIC

The research activity of the “Gas/Solid Interfaces” group has a large and solid background in studying and modelling the interaction of radiation and fast ions with solids, surfaces and nanostructures. In recent years, this research has been devoted to: (i) understand the different mechanisms that determine the reactivity of atoms and small molecules on surfaces and/or nanomaterials, and (ii) predict the outcome of such reactions from first principles. Additionally, the research topics have been extended to the interaction of low-energy molecules with solids and surfaces, performing state-of-the-art molecular dynamics simulations of different physical and chemical processes that take place at surfaces.

HIGHLIGHT

Strong anisotropic interaction controls unusual sticking and scattering of CO at Ru(0001)

Loncaric I, Fuchsel G, Juaristi JI, and Saalfrank P.

Physical Review Letters 119, 146101 (2017)

Molecular beam experiments performed with CO on Ru(0001) showed a quite unusual behavior considering the existing deep adsorption well: incomplete sticking at the lowest incidence energies and narrow scattering angle distributions. In this work, by performing molecular dynamics simulations on a potential energy surface based on first principle electronic structure calculations, the authors reproduce the experimental results and demonstrate that the mentioned unusual behavior is a consequence of a very strong rotational anisotropy in the molecule-surface interaction potential.

Small gas molecules interacting with metal surfaces are of great interest due to their relevance in heterogeneous catalysis. Specifically, the understanding of the interaction of CO with transition metal surfaces is crucial for two catalytic reactions: the oxidation of CO in car exhaust catalytic converters and the Fischer-Tropsch process for which ruthenium is the most efficient catalyst.

Molecular beam experiments have a long standing tradition in surface science and are used to reveal microscopic details about reaction parameters and the potential energy surface. Noticeably, for the important CO/Ru(0001) system the results of these experiments were not fully understood. On the one hand, high sticking probabilities (close to unity) were measured at low incidence beam energies, and a small dependence of the sticking probability on the surface temperature was found. These observations are the evidence for the presence of a deep chemisorption well directly accessible from vacuum without passing an activation barrier. On the other hand, experimental results that are still hard to reconcile with the established picture of a highly exothermic, nonactivated adsorption process were also obtained: sticking was incomplete even at very low incidence energies and, at higher incidence energies, the angular-resolved scattering distributions were found to be surprisingly narrow.

In this work, the authors performed molecular dynamics (MD) simulations that reproduce and explain these intriguing experimental observations. The MD simulations were carried out on a potential energy surface, based on density functional theory calculations. They also allow for the possibility of energy transfer from the molecule to the surface via excitation of surface atom motion and electron-hole pair excitations at the surface region. The study shows that all experimental observations can be rationalized in terms of the strong rotational anisotropy appearing in the CO/Ru(0001) interaction potential. Hence, the work demonstrates the importance of state-of-the-art electronic structure methods and converged, multidimensional dissipative dynamics simulations for the understanding of reactive and nonreactive scattering on catalytic surfaces.

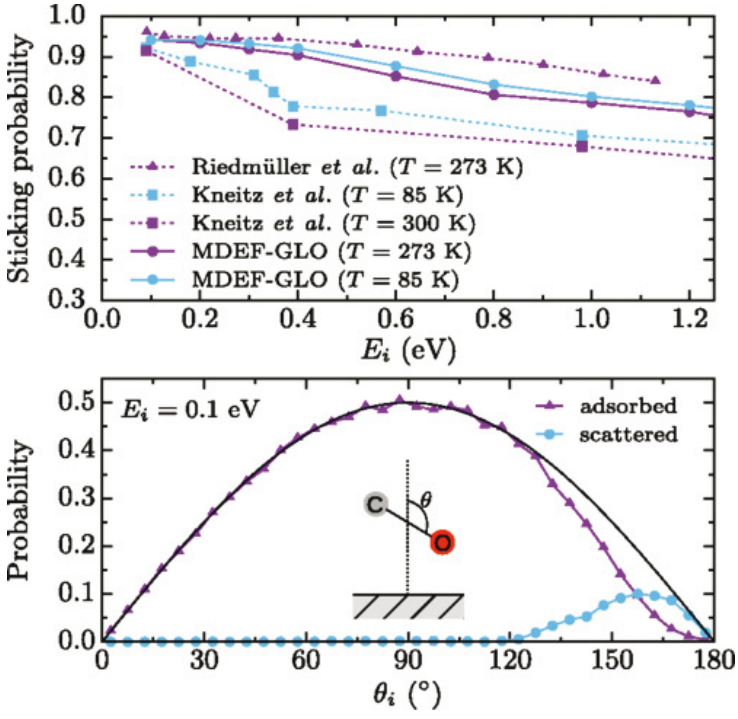


Figure: *Upper panel: Calculated sticking probabilities at normal incidence (solid lines and circles) compared to the experimental results (dashed lines) of S. Kneitz, et al., Surf. Sci. 440, 307 (1999) (squares) and B. Riedmüller, et al, Surf. Sci. 465, 347 (2000) (triangles). Lower panel: Initial orientation θi of scattered (blue circles) and adsorbed (purple triangles) molecules for Ei= 0.1 eV and T = 273 K.*

02

Souza Research Group

The activity of the "Souza Research Group" focuses on fundamental condensed-matter theory, using computational techniques to study the properties of advanced materials from first principles. The activities that the group continues to pursue are: (i) the study of the ground-state, optical, and transport phenomena that arise from broken symmetries such as time reversal (magnetic order) and spatial inversion, and (ii) the description of electronic properties of solids by using geometric phases and related concepts.

In recent years, the work has involved 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 localised Wannier orbitals for metals. Phenomena that arise from the interplay between the collective magnetic order in solids and the spin-orbit interaction inside the constituent atoms have been also successfully addressed.

HIGHLIGHT

Topological pumping of surface anomalous Hall conductivity

Olsen T, Taherinejad M, Vanderbilt D, and Souza I.

Physical Review B 95, 075137 (2017)

The topological pump is a key concept in the field of topological insulators. In the original formulation of Thouless, the Hamiltonian of a one-dimensional (1D) crystal undergoes a slow periodic variation that induces a flow of electrons along the chain. If the chain is insulating (filled bands separated by a gap) the integrated particle current over one cycle amounts to exactly an integer number of electrons. That integer, known as the Chern number C, is a topological invariant characterizing the pump. It can be obtained by integrating the Berry curvature over the 2D-periodic space (k, λ), where k is the wave vector in the 1D Brillouin zone and λ parametrizes the cycle.

The above particle pump in 1D parametric insulators is formally equivalent to the quantization of the transverse (Hall) conductance in 2D Chern insulators: $\sigma_{xy} = C(e^2/h)$, where the Chern number C is now defined in the 2D Brillouin zone (kx, ky), and e^2/h is the quantum of conductance.

In this work, the authors studied a related pumping phenomenon in 3D insulators. Starting from a prototypical model of a 2D Chern insulator known as the Haldane model, a 3D crystal was formed by stacking. The model parameters (intralayer and interlayer couplings) were then modulated periodically. While there was no net flow of electrons over one adiabatic cycle, there was a net flow of Chern number across the slab in the stacking direction , which resulted in the transfer of a quantum e^2/h of anomalous Hall conductivity from the bottom to the top surface.

In the same way that the electron flow in the 1D particle pump can be interpreted as a quantized change in the bulk electric polarization, the Chern-number flow in this 3D Chern pump can be interpreted as a quantized change in the bulk orbital magnetoelectric coupling. In fact, both the electric polarization and the magnetoelectric coupling are only defined as bulk quantities up to a quantum and in order to resolve this indeterminacy one must specify the surface termination.

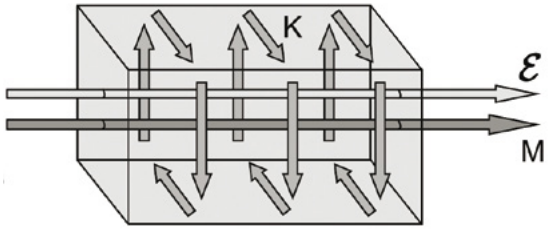


Figure: *Block of material exhibiting an isotropic magnetoelectric coupling. The electric field E induces an orbital magnetization M, which in turns generates circulating currents K on the surfaces. Since the induced surface currents are transverse to the electric field, they can be interpreted as surface anomalous Hall currents.*

03 Nanophysics Lab

The “Nanophysics Laboratory” group joins a team of researchers devoted to a variety of research activities within ultra-high vacuum surface physics. Some of the activities of the group involve: quantum well states in metallic films; electronic states in vicinal surfaces and templates; two-dimensional superlattices; supramolecular self-assembly; physical chemistry in solar cells; and magnetic nanostructures. The general objectives of this research activity within the centre are as follows: (i) to achieve the ultimate, atomic-level control of the electronic and magnetic properties of two- and one-dimensional superstructures, by tuning all growth parameters, namely substrates or molecular units, and (ii) to carry out complementary experiments in ARPES/STM, near ambient XPS, X-ray magnetic circular dichroism (XMCD), X-ray absorption, and Surface X-ray diffraction.

Over the past years, the group has shown expertise in the experimental characterisation of surfaces, low-dimensional systems, and novel nanostructured materials prepared using a surface science approach. The systems have been studied using Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), several photoemission (XPS, ARPES, UPS) and absorption (NEXAFS) techniques, among others. The laboratory has provided a complete structural and electronic characterisation of several nanostructured systems with atomic resolution. The group has also been involved in technological transfer with the creation of a spin-off company, BihurCrystal, connected with the research activity of the laboratory.

HIGHLIGHT

On-surface polymerization onto a rare-earth surface-alloy: towards controlling carbon and rare-earth-based magnetism with atomically tailored nanostructures

Abadia M, Ilyn M, Piquero-Zulaica I, Gargiani P, Rogero C, Ortega JE, and Brede J.

ACS Nano 11, 12392 (2017)

The high reactivity of magnetic substrates toward molecular overlayers has so far inhibited the realization of more sophisticated on-surface reactions, thereby depriving these interfaces of a significant class of chemically tailored organics such as graphene nanoribbons, oligonuclear spin-chains, and metal–organic networks.

The ability to study such *in situ* synthesized structures, which offer an atomic precision of the product with control even over the edge topology, under precisely controlled experimental conditions and in direct contact with a ferromagnetic substrate is of fundamental interest, as it is envisioned as a promising route for studying the many phenomena of emergent carbon-based spintronics by means of spin-resolved measurement techniques offering sub-molecular spatial resolution.

In this work, researchers from the Centro de Física de Materiales (CSIC-UPV/EHU) and Donostia International Physics Center (DIPC), demonstrate the on-surface polymerization of 4,4''-dibromo-*p*-terphenyl precursors into ordered poly(p-phenylene) arrays on top of the surface-alloy GdAu2 (Figure 1). The on-surface reaction is studied employing a multi-technique approach to investigate the chemical, electronic a structural properties of the molecular layer.

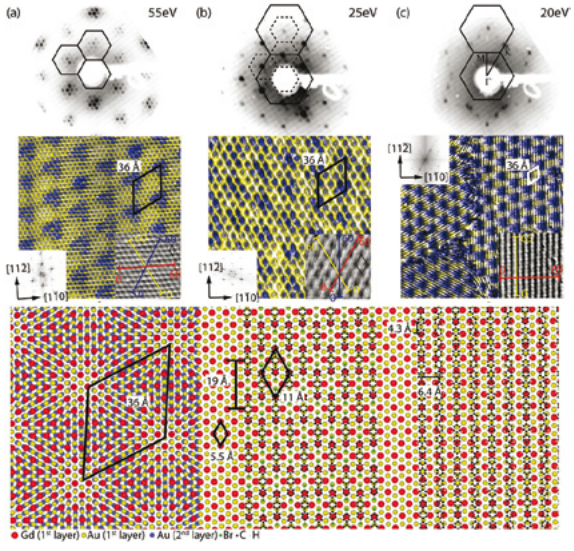


Figure 1: *Low energy electron diffraction (LEED) patterns, scanning tunneling microscopy (STM) topography and structural model of the a) clean surface GdAu2 alloy, b) as-deposited 4,4''-dibromo-p-terphenyl precursors and c) polymerized poly(p-phenylene) molecular nanowires.*

The activation temperatures for bromine scission and subsequent homocoupling of molecular precursors were followed by temperature-dependent X-ray photoelectron spectroscopy. The structural Characterisations of supramolecular and polymeric phases performed by low-energy electron diffraction and scanning tunneling microscopy, establish an extraordinary degree of order extending into the mesoscale. The transition of localized molecular orbitals into a highly dispersive π-band, the fingerprint of successful polymerization, was observed via angular resolved photoemission while leaving all surface-related bands intact. Moreover, employing X-ray magnetic circular dichroism measurements performed at BOREAS beamline(Figure 2) it was possible to demonstrate that although the on-surface reaction alters the magnetic properties of the GdAu2 surface alloy it does not destroy the magnetic order, thus opening the possibility to study carbon-based magnetic nanostructures with atomically-tailored structural properties such as Graphene nanoribbons.

The group acknowledges funding from the Spanish MINECO under contract Nos. MAT2013-46593-C6-4-P and MAT2016-78293-C6-5-R as well as the Basque Government Grants IT621-13 and IT-756-13. J.B. and M.I. are grateful for insightful discussions with Frederik Schiller.

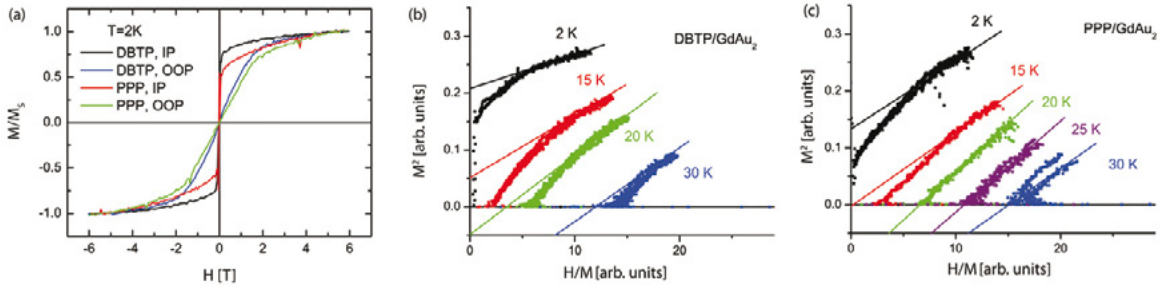


Figure 2: *Magnetic Characterisation performed at BOREAS beamline, a) magnetization loops collected on the as-deposited 4,4''-dibromo-p-terphenyl precursors and polymerized poly(p-phenylene) layer, b) Arrot plots built out of the loops collected on the 4,4''-dibromo-p-terphenyl precursors layer and c) on the poly(p-phenylene) nano-chains.*

Group leader:
Daniel Sánchez
Portal, Scientific
Researcher, CSIC

04 Modelisation and Simulation

The activity of the "Modelisation and Simulation" group focuses on the theoretical study of the electronic and structural properties of complex materials, clean and decorated surfaces, and nanostructures. It pursues the following objectives: (i) to develop the basic theory and ab-initio simulation tools in order to study the behaviour of different nanoelectronic devices, (ii) to study the optical properties of complex organic/inorganic interfaces, (iii) to study magnetism at surfaces, and (iv) to continue to foster the development of the SIESTA code. Most of the research activity of this group is performed in close collaboration with other experimental and theoretical groups in CFM, and also with groups from other research centres in the Basque Country.

In recent years, an important part of this research activity has been devoted to the development of simulation tools, including first-principles simulations of elastic and inelastic transport in nanostructures, and simulations of Scanning Tunneling Microscopy images and tunneling spectroscopies. The group has been also devoted to the study of theory of the interaction of ions and fast particles with solids, surfaces and nanostructures; ultra-fast electron processes and electronic excitations; theory of magnetism in the nanoscale; and TDDFT and many-body perturbation theory methods.

HIGHLIGHT 1

Quantum dots embedded in graphene nanoribbons by chemical substitution

Carbonell-Sanroma E, Brandimarte P, Balog R, Corso M, Kawai S, Garcia-Lekue A, Saito S, Yamaguchi S, Meyer E, Sanchez-Portal D, and Pascual JI.

Nano Letters 17, 50 (2017)

The effect of boron dopants at low concentration on the electronic and transport properties of armchair graphene nanoribbons (aGNRs) with seven dimer lines across their width (7-aGNR) has been studied by a collaboration between the Modelization and Simulation group at CFM and the Nanoimaging group at NanoGUNE. Our study is based on a combination of scanning tunneling spectroscopy (STS) and large-scale density functional calculations using non-equilibrium Green's functions techniques.

Using on-surface synthesis strategies it is possible to grow 7-aGNRs substitutionally doped with diboron (2B) moieties at the centre of the ribbon. In our study we focus on regions where the 2B centres are separated by several nanometers. Besides impurity levels localized around the 2B centres, in the pristine regions between two 2B centres, we find clear signatures of the quantization of some of the 7-aGNR bands. Theoretical calculations have been instrumental to understand the origin of the quantized levels in detail.

Figure a shows a scheme of one the studied systems, composed by 2B defects situated 6.5 nm apart. Figure e shows the corresponding STS results. Besides the 2B-defect levels at ~-0.5 eV and ~-1.8 eV, one can see resonances at well-defined energies extending over the whole pristine region between the defects. They were tentatively assigned to quantum well states (QWSs) coming from the bands of the pristine 7-aGNR. Figure c shows the corresponding projected density of states (PDOS) from density functional calculations. Except for small energy shifts of the levels, the favourable comparison between theory and experiment is evident. The calculations confirm the number and approximate energy location of the localized 2B-defect levels, as well as the presence of QWSs.

Figure b shows the computed electron transport characteristics. These results show the enhanced transport at the energies corresponding each QWS. This effect is similar to that of Fabry-Perot resonances in optics. Figure b clearly indicates that the QWSs are derived from the valence band (VB) of the 7-aGNR. In contrast, the lower valence minus one (VB-1) band is almost immune to scattering at the 2B impurities. This is further confirmed by the inspection of the transmission eigenchannel wavefunctions in Figure d. The different behaviour can be traced back to the different symmetry of both bands. The VB has even symmetry across the ribbon and interacts strongly with the 2B-derived defect states appearing at higher energies. In contrast, the VB-1 presents a node in the centre of the ribbon and it is only weakly affected by the 2B defects. Similar differences take place between the conduction (CB) and CB+1 bands.

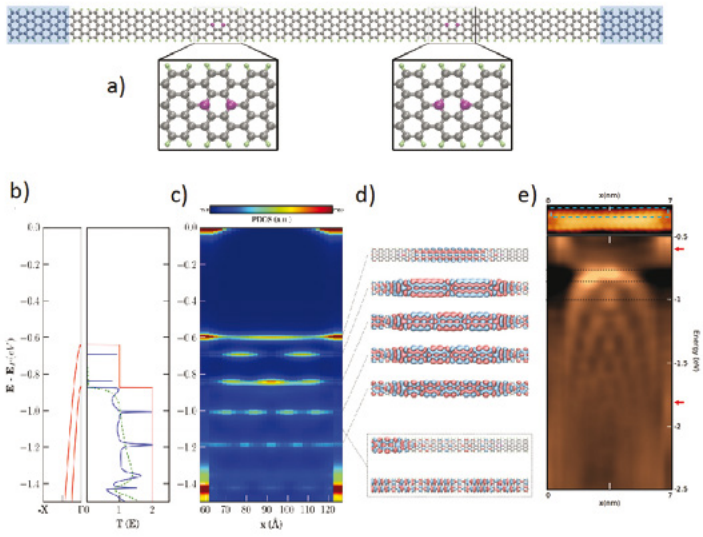


Figure: *a) Model of the studied system formed by a pristine 7-aGNR region enclosed by two 2B-defects 6.5 nm apart. b) Dispersion of the VB and VB-1 bands of a pristine 7-aGNR, (left) and transmission function (right) for a pristine ribbon (red), a single boron pair (dashed green) and for the confined system formed by two boron pairs (blue). c) Projected density of states for the pristine segment. Quantized levels up to n=5 are clearly observed between the boron localized states. d) Real part of the eigenchannel functions taken at the energies corresponding to the n=2, 3, 4 and 5 QW levels. In the dashed panel are presented the real part of the eigenchannel functions taken at E-EF=-1.10 eV, i.e. between quantized levels. The eigenchannel corresponding to the VB shows no transmission through the boron segments, while VB-1 fully transmits through. e) Experimental results obtained using scanning tunneling spectroscopy.*

HIGHLIGHT 2

Electric-field-driven direct desulfurization

Bogdana Borca, Tomasz Michnowicz, Rémi Pétuya, Marcel Pristl, Verena Schendel, Ivan Pentegov, Ulrike Kraft, Hagen Klauk, Peter Wahl, Rico Gutzler, Andrés Arnau, Uta Schlickum, and Klaus Kern

ACS Nano 11, 4703 (2017)

A collaboration with the experimental group of Prof. Klaus Kern at the Max Planck Intitut in Sttutgart has permitted us to explore chemical reactions implying the dissociation of carbon-sulfur bonds, which are fundamental for understanding the carbon and sulfur cycles in nature. Additionally, desulfuration reactions are of industrial significance in processes aimed at cleaning natural fuels. However, a clear understanding of desulfuration reaction at the submolecular level, including the identification of the reaction paths, is a challenging problem.

In this work, we track the chemical pathway of an irreversible direct desulfurization reaction of tetracenothiophene adsorbed on the Cu(111) closed-packed surface at the submolecular level. Using

the precise control of the tip position in a scanning tunneling microscope and the electric field applied across the tunnel junction, the two carbon–sulfur bonds of a thiophene unit are successively cleaved. Comparison of spatially mapped molecular states close to the Fermi level of the metallic substrate acquired at each reaction step with density functional theory calculations reveals the two elementary steps of this reaction mechanism. The first reaction step is activated by an electric field larger than 2 V nm–1, practically in absence of tunneling electrons, opening the thiophene ring and leading to a transient intermediate. Subsequently, at the same threshold electric field and with simultaneous injection of electrons into the molecule, the exergonic detachment of the sulfur atom is triggered. Thus, a stable molecule with a bifurcated end is obtained, which is covalently bound to the metallic surface. The sulfur atom is expelled from the vicinity of the molecule.

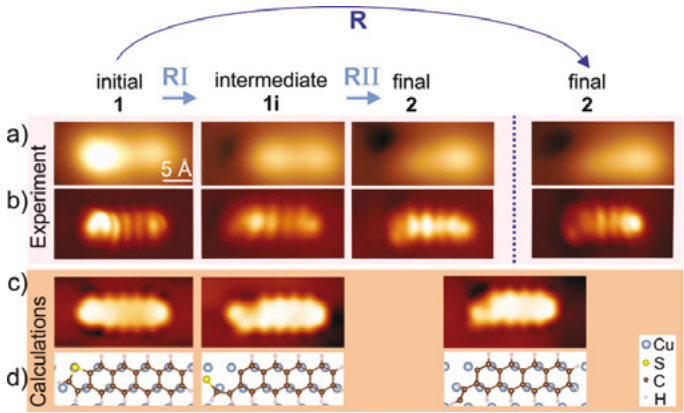


Figure: *Molecular conformations at each stage of the direct desulfurization reaction obtained by STM investigations and DFT calculations. a) Topographic images acquired in constant current mode. The reaction R represents the reaction that directly transforms the system from state 1 to the final state 2. The reactions RI and RII represent the two steps of the desulfurization process, from the initial state 1 to the intermediate state 1i and from 1i to the final state 2. b) Spatial maps of the molecular states obtained with a functionalized tip, acquired in constant height mode (I = 100 pA, V = –1 V left image, I = 100 pA, V = 100 mV all other images). c) Molecular appearances in the Tersoff–Hamann approximation obtained from DFT-vdW simulations for each molecular state. d) Ball-and-stick representation of the calculated molecular sequences on the Cu(111) surface (top views).*

Group leader: Lucia Vitali, Ikerbasque Professor, UPV/EHU

05 Spectroscopy at Atomic Scale

The activity of the "Spectroscopy at Atomic Scale" group is devoted to explore the structural and spectroscopic characteristics of materials at the local scale, with the use of Scanning Tunneling Microscopy (STM) techniques. The objectives of this activity have been essentially focused on: (i) the understanding of different mechanisms that influence the electronic, magnetic and vibrational properties on surfaces, (ii) the study of electron transport and chemical reactivity of surface supported nanostructures, and (ii) the investigation of new strategies leading to the formation of covalently- bonded conjugated structures with functional groups.

Over the past years, the group has been especially dedicated to install a low temperature scanning probe microscope. This is the main tool that has been used for studying nanostructures at the atomic scale. Thus, local properties of nanoscale objects and surfaces have been probed in ultra-high vacuum and at temperatures down to 1K, a challenging situation from the methodological point of view.

HIGHLIGHT

Self-texturizing electronic properties of a 2-dimensional GdAu2 layer on Au(111): the role of out-of-plane atomic displacement

Correa A, Camellone MF, Barragan A, Kumar A, Cepek C, Pedio M, Fabris S, and Vitali L.

Nanoscale 9, 17342 (2017)

The authors demonstrate the spontaneous texturing of the electronic and chemical properties of a 2-dimensional layer GdAu2 on Au(111) as a consequence of layer-buckling and out-of-plane atomic displacement.

One of the major issues of nanoscience and technology is the patterning of electronic properties and chemical reactivity of 2-dimensional layers at nanoscale. Researchers of CFM in collaboration with the CNR-IOM-Trieste have demonstrated that the electronic properties of a weakly interacting 2-dimensional layer can spontaneously texturize. The two fundamental parameters that allow achieving the desired periodic modulation are the variable adsorption stacking configurations and structural relaxation processes. Interfaces characterized by mismatched two-dimensional layers in weak interaction are expected to be an excellent playground to template the electronic structure and chemical reactivity. Notwithstanding that such geometrical configurations are commonly observed in Moiré superstructures, little attention has been paid on the effect of layer-buckling on the electronic properties. Here, the team has investigated the induced periodic modulation of the electronic properties by scanning probe techniques and theoretical modeling to gain insights into the correlation between its electronic properties and layer planarity.

Specifically, a monolayer of a bi-metallic alloy, namely GdAu2, obtained upon evaporation of gadolinium atoms on the annealed Au(111) surface has been characterized. This results in a weakly interacting Moiré superstructure, characterized by a variable adsorption stacking configuration. This induces a layer-buckling at the GdAu2/Au(111) interface and modulates the electronic properties and chemical reactivity of the system. The layer/substrate coupling and the induced out-of-plane displacement of the Gd atoms is sufficient to locally open an energy gap of 0.5 eV at the Fermi level in an otherwise metallic layer. Additionally, this buckling changes the character of the hybridized Gd-pd and Au-sp states and controls the energy of the occupied and unoccupied Gd 4f multiplet proportionally to the lattice distortion. We demonstrate that the resulting template shows different chemical reactivity, which may find important applications.

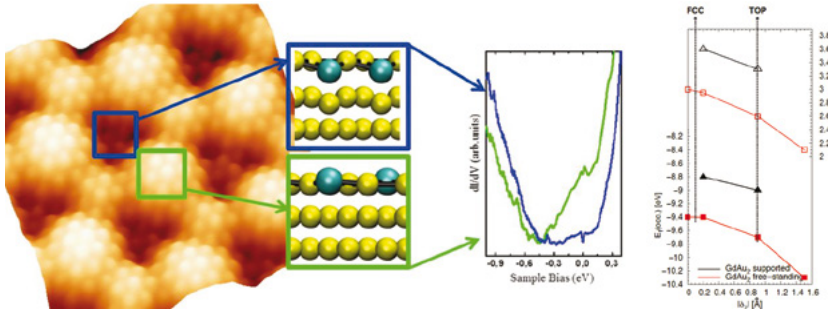


Figure: *3D topographic image of the GdAu2/Au(111) forming a Moiré pattern and theoretical modeling of the variable out-of-plane atomic relaxation. As a consequence of this layer buckling, the electronic properties of the layer are patterned from the Fermi level to the Gd4f states.*

ELECTRONIC PROPERTIES AT THE NANOSCALE

The research line "Electronic Properties at the Nanoscale" focuses on the theoretical investigation of electronic properties of solids, surfaces, nanostructures, and low-dimensional systems. Research within these topics has tackled the electronic properties of both ground and excited states of these systems, in particular, the electronic response of materials under different perturbations. Different experimental probes are investigated in this research line: electromagnetic radiation, electrons, ions, etc. Size and border effects, as well as the dimensionality of nanosized materials are studied as a means to change their properties.

Five research groups develop the activities of this theoretical research line. The activity of all these groups covers the study of a wide range of advanced materials at microscopic and mesoscopic scales, based on state-of-the-art methodologies. Some of the materials studied show special conditions of interest in a particular subfield of interest, such as materials under high pressure, spintronics, nanomagnetism, or attosecond dynamics in solids. The list of activities developed by the different groups with their corresponding highlights follows:

06 Electronic Excitations in Surfaces and Nanostructures

Group leader: Andrés Ayuela Fernández, Scientific Researcher, CSIC

The activity of the "Electronic Excitations in Surfaces and Nanostructures" group is devoted to the theoretical study of electronic and magnetic properties of solids, surfaces and low-dimensional systems, particularly focusing on systems of nanometer size. The general interests of this activity include: (i) spin dependent electronic excitations in metals, (ii) electronic states and excitations in topological insulators, (iii) many-body theory of electrons lifetimes, (iv) basic properties, such as energy dispersion and lifetimes of novel low-energy collective excitations, and (v) nanostructures of carbon nanotubes, inorganic nanotubes and minerals with silicate chains.

06 ELECTRONIC EXCITATIONS IN SURFACES AND NANOSTRUCTURES

In recent years, electronic and magnetic properties of materials have been investigated using first principles methodologies in this research line. Electron dynamics in different systems have been also studied, with particular emphasis on ultrafast processes and size effects. Advanced materials, such as topological insulators and cement-related systems, are current targets of these activities.

HIGHLIGHT

Angular momentum induced delays in solid state photoemission enhanced by intra-atomic interactions

Siek F, Neb S, Bartz P, Hensen M, Struber C, Fiechter S, Torrent-Sucarrat M, Silkin VM, Krasovskii EE, Kabachnik NM, Fritzsche S, Muino RD, Echenique PM, Kazansky AK, Muller N, Pfeiffer W, and Heinzmann U.

Science 357, 1274 (2017)

Even more than 100 years after Einstein's explanation of photoemission the process of electron emission from a solid material upon illumination with light still poses challenging surprises. In our work, ultrashort pulses of light were employed to start a race between electrons emitted from different initial states in a solid material. Timing this race reveals an unexpected result: The fastest electrons arrive in last place.

Experimentally resolving the tiny delays in a photoemission process required timing the emission event, i.e. the moment when the electron leaves the material, with an unprecedented resolution of 10-17 seconds. This hardly conceivable resolution allows timing the race of electrons in experiments that were performed at Bielefeld University (Germany) using advanced attosecond time-resolved laser spectroscopy. The choice of tungsten diselenide as material from which the photoemission takes place turned out to be essential: It provides four photoelectron emission channels with different initial state properties and the outstanding stability of the surface enabled long-term data collecting improving the statistical significance.

The explanation and theoretical modelling of the electron race outcome was made by a team of physicists from the Centro de Física de Materiales (CSIC-UPV/EHU) and the Donostia International Physics Center (DIPC). The motion of a photoemitted electron is strongly affected by interactions inside the atom from which the electron is emitted. Electrons photoemitted from a surface remain trapped for a while, dynamically confined by the centrifugal barrier around the atoms. The motion of these electrons around the nuclei, before being eventually emitted, is kind of a dance leading to an intuitive picture that the electrons that remain longer dancing around the atom lose the race and are emitted last.

Still the achieved theoretical model represents just a first step in the interpretation of the measured electron race since intra-atomic motion and propagation in the crystal are treated separately. In the future these processes shall be treated in a unified approach and the thus improved theory of photoemission will open new possibilities to experimentally test and improve our understanding of the very fundamental process of photoemission. Control of light with attosecond (10 -18 second) resolution opens fascinating views on electron dynamics on the atomic scale. Whereas femtosecond (10-15 second) spectroscopy served to study and control atomic motion, attosecond spectroscopy now directly addresses the fundamentals of the interaction of light with matter.

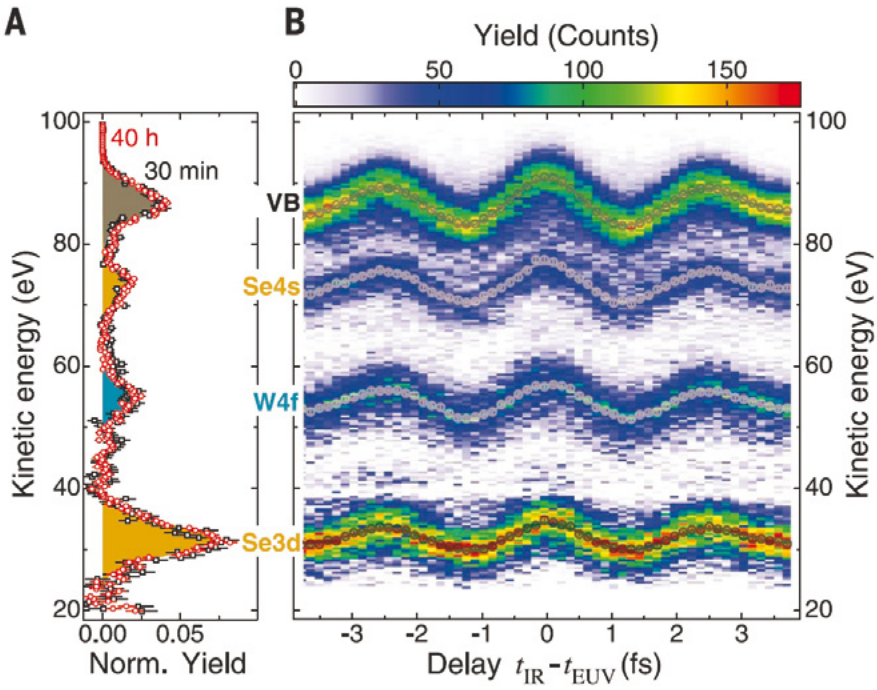


Figure: *Attosecond time-resolved photoemission spectroscopy from WSe2. (A) Long-term stability of the surface over 40 hours. Background-corrected photoemission spectra recorded 30 min (black circles) and 40 hours (red circles) after cleaving. The photoelectron peaks for VB, Se 4s,W 4f, and Se 3d are indicated. The spectra are normalized to the total yield after background subtraction. (B) Streaking spectrogram. As a function of the delay between the IR and EUV pulses, the photoemission spectra (after background subtraction) are shown as a density plot. For each delay, the energy positions (overlaid symbols) of the VB, Se 4s, W 4f, and Se 3d emissions and the corresponding simultaneously fitted IR field-time dependence yielding the delay parameters Dt for each emission channel (continuous overlaid lines) are shown.*

07 Materials Computation and Theory

The activity of the "Materials Computation and Theory" group focuses on the first-principles calculation of the electronic structure of materials under extreme conditions of pressure and temperature, as well as superconductivity. This approach serves to analyse and understand the optical, electronic and magnetic properties, as well as superconductivity of special materials, and the environmental conditions which determine special electronic properties. Ab-initio approximations are used in this case to solve interesting puzzles in special materials and surface science.

Over the past years, the activity on this topic has been especially dedicated to: (i) clarify if hydrogen or other hydrogen rich hydrides may be room temperature superconductors at megabar pressures, (ii) study time-dependent density-functional theory beyond the local-density approximation, (iii) characterise collective excitations, and (iii) study optical lattices.

HIGHLIGHT

Pressure-induced stable Li5P for High-Performance Lithium-ion batteries

Zhao ZY, Liu LL, Yu T, Yang GC, and Bergara A.

Journal of Physical Chemistry C 121, 21199 (2017)

In order to find high-capacity anode materials for Li-P batteries the authors analyzed Li-P compounds by employing unbiased structural search and found two novel phases, Fm-3m Li3P and P6/mmm Li5P, stable above 4.2 GPa and 10.3 GPa, which might be quenching recoverable to ambient conditions.

Black phosphorus, the result of white P under high pressure, has received much attention as a promising anode material for Li-ion batteries (LIBs). However, the final product of lithiation, P63/mmc Li3P, is not satisfactory due to its poor conductivity. In this article we explore the high-pressure phase diagram of the Li-P system through first-principles swarm-intelligence structural search and present two hitherto unknown stable Li-rich compounds, Fm-3m Li3P at 4.2 GPa and P6/mmm Li5P at 10.3 GPa. Metallic Li5P exhibits interesting structural features, including graphene-like Li layers and P-centered octadecahedrons, where P is 14-fold coordinated with Li. Interestingly, both compounds exhibit good dynamical and thermal stability properties at ambient pressure, and the theoretical capacity of P6/mmm Li5P reaches 4326 mAhg-1, the highest among the already known Li-P compounds. Additionally, their mechanical properties are also favorable for electrode materials. Our work represents a significant step towards the performance improvement of Li–P batteries and understanding Li-P compounds.

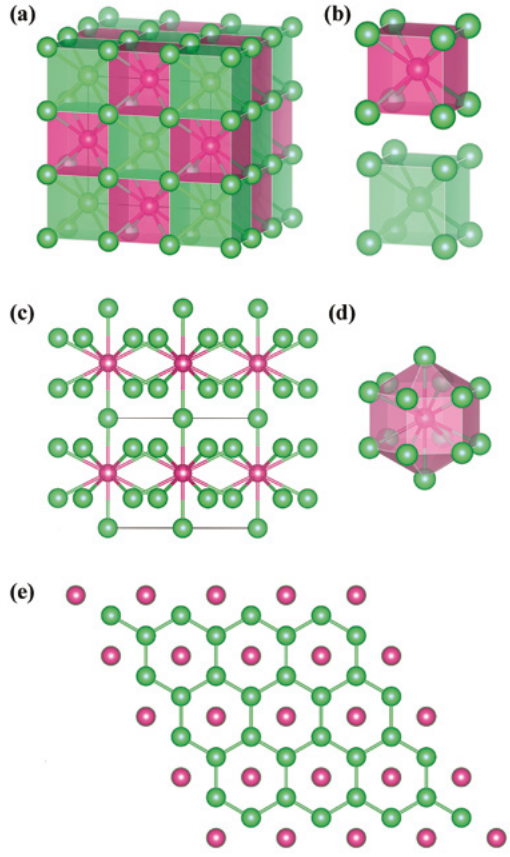


Figure: *Structural features of Fm-3m Li3P and P6/mmm Li5P at 0 GPa. (a) Li3P in the Fm-3m structure. (b) Coordination environment of P and Li atoms in Li3P. (c) Li5P in the P6/mmm structure. (d) Coordination environment of the P atom in Li5P. (e) P6/mmm structure of Li5P viewed along the c-axis. In all the structures, green and pink spheres represent Li and P atoms, respectively.*

Group leader:
Sebastián Bergeret
Sbarbaro, Tenured
Scientist, CSIC

08 Mesoscopic Physics

The activity of the "Mesoscopic Physics" group is devoted to the theoretical study of the properties of mesoscopic systems consisting of metals, ferromagnets, semiconductors, superconductors, cold-atoms systems, organic materials and topological insulators. Especial emphasis is placed on electronic transport, pursuing the following objectives: (i) the study of spin transport in superconductor/ferromagnet and semiconducting structures, (ii) the investigation of heat transport in nanostructures and design of thermoelectric elements at the nanoscale, (iii) the study of the dynamics of phase coherent effects in mesoscopic systems, and (iv) the theoretical study of strongly correlated and low dimensional systems. Additionally, applications for nanoelectronics, spintronics and caloritronics are also studied and several collaboration projects have been designed with top universities in the USA to launch joint initiatives. A good example is the joint workshop on "Frontiers in Quantum Materials & Devices" with the University of Harvard celebrated in Donostia-San Sebastián in July 2017.

In recent years, the group has been particularly focused on the development of theoretical frameworks to describe several phenomena related to quantum transport in mesoscopic systems, aiming at applying the results obtained in the performance of nanodevices.

HIGHLIGHT

Revealing the magnetic proximity effect in EuS/Al bilayers through superconducting tunneling spectroscopy

Strambini E, Golovach VN, De Simoni G, Moodera JS, Bergeret FS, and Giazotto F.

Physical Review Materials 1, 054402 (2017)

The authors demonstrate a robust exchange splitting of the density of states of superconducting Al adjacent to a EuS layer. Such spin-splitting appears even in the absence of an external magnetic field. Our findings place EuS/Al as the most suitable material combination for different applications.

Superconductors with spin-split density of states are essential for the emerging field of superconducting spintronics, topological quantum computation, cryogenic RAMs and ultra-sensitive thermoelectric sensors. All these applications need a sizeable splitting of the superconducting density of states in a large temperature range below the critical temperature. In principle spin-splitting can be achieved by applying large magnetic fields to thin superconducting layers. However, it is well known that magnetic fields weaken superconducting properties. A way to overcome this problem is to place a ferromagnetic insulator adjacent to a superconducting layer: Electrons form the latter may interact with the localized spins of the insulator and being polarized. This will lead to a spin-polarized density of states which can be measured by tunnel spectroscopy.

This collaboration between Sebastián Bergeret and Vitaly Golovach from the "Mesoscopic Physics" group at the CFM, and the groups of Francesco Giazotto (CNR Italy) and Jagadeesh Moodera (MIT, USA) demonstrates a clear exchange splitting in EuS/Al bilayers, which is observed even in the unmagnetized state of the EuS layer (see Figure). The measurements and theoretical modelling suggests that the domain size of the EuS is comparable with the superconducting coherence length. For that reason this material combination is the proper platform for development of the above mentioned application.

Specifically, this work is pivotal in fabricating the ultra-sensitive thermoelectric bolometers proposed and designed by the Mesoscopic Phsyics Group at the CFM and collaborators.

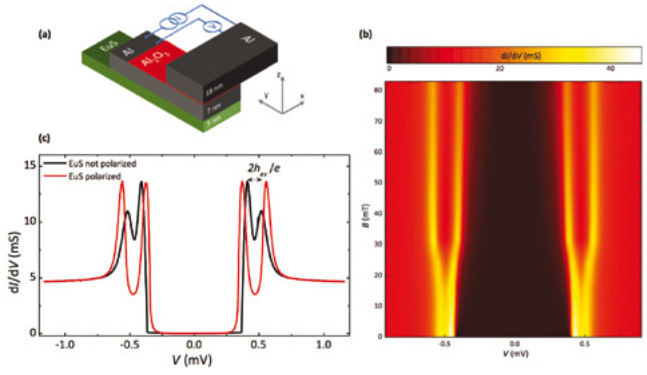


Figure: *a) Sketch of the cross bar EuS(5)/Al(7)/Al2O3/Al(18) vertical tunnel junction studied in our work (thickness in nanometers). b) Evolution of the differential conductance, as a function of the voltage drop (V) and in-plane magnetic field (B) during the first magnetization of the EuS layer. c) Comparison between the differential conductance of the tunnel junction measured at zero field before (black curve) and after (red curve) the magnetization of the EuS layer. All the measurements done at 25 mK.*

Group leader: Ángel Rubio Secades, University Professor, UPV/EHU

09 Nano-Bio Spectroscopy

The activity of the "Nano-Bio Spectroscopy" group is devoted to the field of theory and modelling of condensed matter electronic and structural properties, with special emphasis in the optical response of nanosystems. A strong program focusing on developing novel theoretical tools and computational codes to investigate the electronic response of solids and nanostructures to external electromagnetic fields has been settled in this group. The main research interests of this activity are as follows: (i) foundations of time-dependent density functional theory for biophysics, (ii) foundations of many-body theory, (iii) electronic and thermal transport, (iv) theory of open quantum systems, (v) strong light-matter interactions and optimal control theory.

In recent years, the main research activities on this topic include new developments within many-body theory and TDDFT, covering ab-initio description of electron excitations, optical spectroscopy, time-resolved spectroscopies, and lifetimes. Novel techniques to calculate total energies haven been also developed, assessing exchange correlation (XC) functionals for TDDFT calculations. Improvements on transport theory within the real-time TDDFT formalism have been also achieved. Moreover, the electronic and optical properties of solids, nanostructures (in particular nanotubes, nanowires and semiconducting -clusters-) and biomolecules is also tackled in the group. All these activities have resulted in the establishment of the European Theoretical Spectroscopy Facility (ETSF).

HIGHLIGHT

Creating stable Floquet-Weyl semimetals by laser-driving of 3D Dirac materials

Hubener H, Sentef MA, De Giovannini U, Kemper AF, and Rubio A.

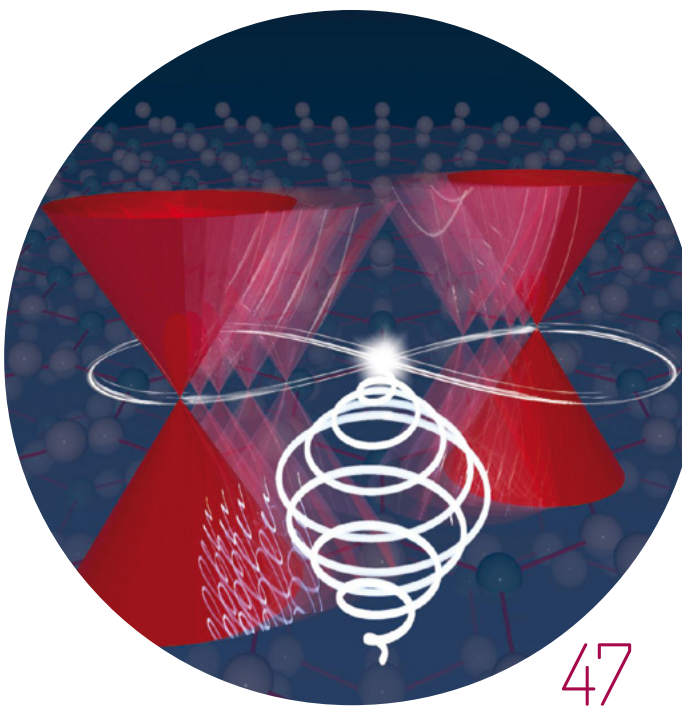
Nature Communications 8, 13940 (2017)

Laser-driving of semimetals allows creating novel quasiparticle states within condensed matter systems and switching between different states on ultrafast time scales. Studying properties of fundamental particles in condensed matter systems is a promising approach to quantum field theory. Quasiparticles offer the opportunity to observe particle properties that have no realization in elementary particles

In the present study, an international research team led by Angel Rubio from the Max Planck Institute for the Structure and Dynamics of Matter at CFEL in Hamburg and the University of the Basque Country in Donostia-San Sebastián predicted how laser light can be used to create Weyl fermion states in 3D Dirac materials and to switch between Weyl semimetal, Dirac semimetal and topological insulator states on ultrafast timescales. Besides its relevance for fundamental quantum physics, the results might lead to applications in ultrafast switching of material properties. The findings are published online in the journal Nature Communications today.

In the standard model of particle physics, the fundamental particles that make up all matter around us – electrons and quarks – are so-called fermions, named after the famous Italian physicist Enrico Fermi. Quantum theory predicts that elementary fermions could exist as three different kinds: Dirac, Weyl, and Majorana fermions, named after Paul Dirac, Hermann Weyl, and Ettore Majorana. However, despite being predicted almost a hundred years ago, of these three kinds of particles only Dirac fermions have been observed as elementary particles in nature so far. With the discovery of graphene in 2004, however, it was realized that the behaviour of relativistic free particles could be observed in the electronic properties of materials. This sparked the search for materials where these fundamental particles could be observed and only last year the first materials hosting Weyl fermions were discovered. While any known material only hosts one kind of these fermions in its equilibrium state, in the present work it is demonstrated how one can transform the fermion nature within specific materials by using tailored light pulses.

Figure: *Dancing Weyl cones: When excited by tailored laser pulses (white spiral), the cones in a Dirac fermion material dance on a path (8-shape) that can be controlled by the laser light. This turns a Dirac material into a Weyl material, changing the nature of the quasiparticles in it. One of the cones hosts right-handed Weyl fermions; the other cone hosts left-handed ones. © Jörg M. Harms/MPSD.*



Group leader: Nicolás Lorente Palacios, Scientific Researcher, CSIC

10 Quantum Phenomena on Surfaces

The activity of the "Quantum Phenomena on Surfaces" group focuses on the development of computational schemes to unveil the richness of realistic spectral functions. The main research topics in the group are electronic, vibrational and magnetic excitations, particularly of molecular and nanomagnetic systems on surfaces.

In recent years, the following objectives have been addressed on these topics: (i) the use of density functional theory to understand the geometrical and electronic structure of different surface systems, and (ii) the development of theories and numerical treatments to understand phenomena revealed by the STM. This activity has been awarded during 2017 with a European FET Open project in the H2020 framework, where the Donostia-San Sebastián node is led by this group.

HIGHLIGHT

Building complex Kondo impurities by manipulating entangled spin chains

Choi DJ, Robles R, Yan SC, Burgess JAJ, Rolf-Pissarczyk S, Gauyacq JP, Lorente N, Ternes M, and Loth S.

Nano Letters 17, 6203 (2017)

The Kondo effect is an exotic process revealing the many-body character of quantum matter at low temperatures. At higher temperatures, one-particle excitations set it and the collective properties of correlated ground states are not accessible.

Creating many-body states is of great interest to understand correlations among particles in the quantum world. In this work, D.-J. Choi in collaboration with a group in Hamburg, and theoreticians in Stuttgart, Orsay and Donostia, created a complex system by manipulating atoms on a copper nitrate surface. Initially they used Mn atoms. These atoms do not form a Kondo state. In order to form a Kondo states, the adatom must be magnetic and have a degenerate ground state that only differ in a spin flip. In this way, the contact with metal electrons, creates a virtual current of electrons changing their spin at the same time as the magnetic adatom changes its ground state. This leads to a strongly correlated many-body ground state of the full adatom-substrate system. Then they used Fe atoms, that do not form Kondo states either. However when they created dimers of FeMn on the copper nitrate surface, the Kondo state was formed! Moreover, long chains of Mn atoms ending on a single Fe atom would present a Kondo state. But long chains of Fe atoms ending on a single Mn did not present Kondo state. These findings could be rationalize in terms of the magnetic anisotropy of the different constituents and in the interactions between atoms. Mn chains have a strong interatomic interaction but weak anisotropy, so that their spin can be easily changed. When adding a Fe atom a degenerate ground state was created that could be flipped by a metal electron. Then the Kondo effect appears. However, Fe chains have a large magnetic anisotropy that prevents changing the chain spin.

This work shows that exotic many-body states can be created by using single-atom manipulation and by understanding the characteristics of the different constituents of matter.

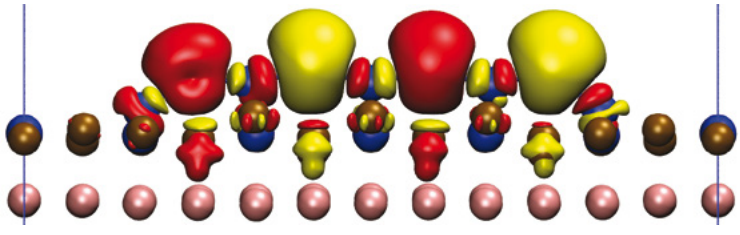


Figure: *Spin electronic density showing the different magnetic moments of electrons over a FeMn3 chain made on a copper nitrate surface (blue atoms are N atoms and pink ones are Cu atoms). This distribution shows the strong interaction between magnetic atoms mediated by the non-magnetic N atoms in a superexchange-like scheme.*

PHOTONICS

The research line on "Photonics" deals with the experimental and theoretical study of the interaction of radiation with matter from different and complementary approaches: (i) the interaction of light with metallic and semiconductor nanostructures to confine and engineer electromagnetic fields in the nanoscale, (ii) 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) spectroscopy and photonic applications of nano-scale functional units, including different types of low-dimensional systems. Several research activities along these lines are developed by the groups listed below, including theoretical and experimental activities.

During 2017, a new group in the research line of Photonics has been launched at CFM, with a focus on the experimental study of the interaction of non-classical states of light with nanostructures, the "Quantum Nanophotonics Laboratory", led by Ikerbasque Professor Gabriel Molina Terriza who joined CFM in June 2017.

11

Theory of Nanophotonics

Group leader: Javier Aizpurua Iriazabal, Research Professor, CSIC

The activity of the "Theory of Nanophotonics" group is devoted to the theoretical study of the interaction between electromagnetic radiation and nanostructured materials. The research activity of the group focuses on the theoretical study of the excitation of plasmons, quantum dots and dielectric nanostructures in the context of a variety of microscopy and spectroscopy techniques: Dark Field Microscopy (DFM), scattering-type Scanning Near-Field Optical Microscopy (s-SNOM), Electron Energy Loss Spectroscopy (EELS), Scanning Tunneling Microscopy (STM), Surface-Enhanced Raman Scattering (SERS), Surface-Enhanced

Infrared Absorption (SEIRA) and Surface-Enhanced Fluorescence (SEF), among others.

In recent years, the following specific objectives have been addressed on this topic: (i) understanding and characterisation of the collective excitations of the electron gas, plasmons, in a variety of spectroscopy and microscopy techniques, (ii) study of metallic nanostructures as electromagnetic field enhancers and localizers, (iii) development of protocols and models to better interpret and describe the images obtained by the scattering-type near-field optical microscope, (iv) study and exploitation of the interaction of fast electrons and matter to develop new paradigms of spectroscopy in the nanoscale, (v) description of quantum effects derived from the coherent nature of the electrons that constitute a plasmonic excitation, (vi) study of the magnetic activity of dielectric nanostructures at optical frequencies, and (vii) characterisation of the dynamics and the coupling of emitters to be used in quantum information technology.

HIGHLIGHT

Coherent interaction between a single molecule and a plasmonic cavity

Zhang Y, Meng QS, Zhang L, Luo Y, Yu YJ, Yang B, Zhang Y, Esteban R, Aizpurua J, Luo Y, Yang JL, Dong ZC, and Hou JG.

Nature Communications 8, 15225 (2017)

Light emission from a single molecular emitter can be modified when the molecule is located close to a plasmonic cavity. By controlling the position of the molecule in the cavity of a Scanning Tunneling Microscope within Ångstrom precision, molecular electroluminescence can be monitored revealing interference patterns. A theoretical model that considers the electromagnetic interaction between molecular dipole and plasmonic cavity reproduces the Fano spectral profiles and Lamb shifts experimentally observed.

Light confined into plasmonic cavities of nanometer size interacts very efficiently with single molecules, allowing for accessing and manipulating their electronic states. Surface plasmons, the collective resonances of the free electrons at metallic interfaces, are able to trap light into tiny effective mode volumes, dramatically enhancing the interaction between photons and molecular excitations. By exciting a very small plasmonic hot-spot in the cavity formed in a metallic STM tip and a substrate, an exquisite control of the coherent interaction between a plasmonic cavity and a single molecule has been demonstrated.

The “Theory of Nanophotonics” group at the Center for Materials Physics (CFM) and the Donostia International Physics Center (DIPC) in Donostia-San Sebastián, together with experimental collaborators at the University of Science and Technology of China in Hefei, have

studied theoretically and experimentally the optical response of a molecule located in the proximity of a silver STM tip at cryogenic temperature. The molecule is deposited on a silver substrate covered by a NaCl monolayer avoiding chemical interaction. The tip-substrate system forms a natural plasmonic cavity that confines electromagnetic energy into a small plasmonic hot-spot at the gap. The tunneling current between the tip and the metallic substrate allows for controlling and monitoring the lateral position of the tip with respect to the molecule within subnanometer resolution.

When the molecule is deposited under the tip, the tunneling current directly excites the electronic transitions of the molecule, which emits very efficiently due to its coupling with the plasmon resonance. An even more interesting situation occurs when the molecule is slightly displaced out of the plasmonic cavity (Figure a). In such a situation, the tunneling current excites the plasmonic resonance, which boosts the molecular transition, giving rise to an electromagnetic interaction between them. This coherent 'back-and-forth' interaction between molecule and plasmonic cavity results in a characteristic Fano profile of the light emitted (Figure b).

By tracing the changes in the Fano profile of light emission as the tip is displaced with respect to the molecule, a strong localization of the electromagnetic field of ≈1nm lateral size within the plasmonic cavity can be identified. The molecular exciton-plasmon interaction can reach strong values of the coupling strength, producing a 10,000 fold increase of the rate of molecular emission (Purcell effect). Furthermore, this interaction also leads to changes in the energy of the molecular transition as large as ≈1nm (3meV) due to the so-called photonic Lamb shift. This work thus advances towards the control of electronic states of individual molecules by coherent coupling with plasmonic modes.

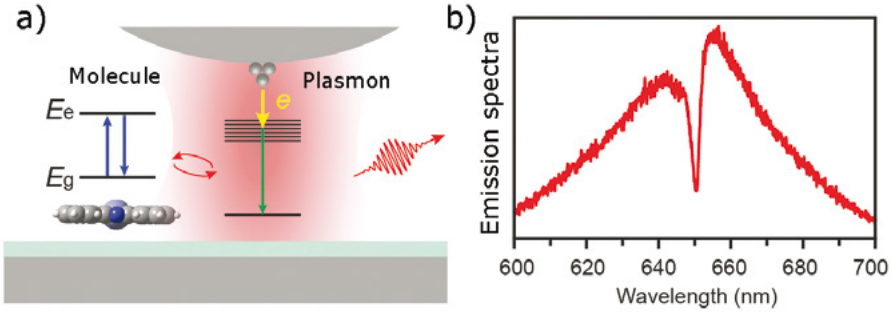


Figure: *(a) Schematics of the molecule-plasmon system realized in a STM cavity. An electron current between the metallic tip and substrate (depicted by the yellow arrow) excites a plasmonic cavity resonance (represented by the ground state and the quasi-continuum of states at the centre of the figure, with the green arrow depicting the plasmonic decay). The cavity plasmon interacts with a two level transition of a molecule (characterized by a ground state Eg and an excited state Ee) resulting in the emission of a photon. The corresponding light emission spectrum is shown in (b) for a situation with the molecule laterally close to the STM plasmonic cavity.*

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

12 Nanomaterials and Spectroscopy

The activity of the "Nanomaterials and Spectroscopy" group focuses on the experimental study of spectroscopy and photonic applications of nano-scale functional units, including semiconductor quantum dots and quantum wires, metal nanoparticles and nanoantennas, as well as organic/inorganic nano-hybrid systems. A nanophotonics laboratory, where lifetime microscopy based on fluorescence emission spectroscopy is the fundamental equipment, allows this activity.

Over the past years, the research on this topic has targeted the following specific objectives: (i) the development of novel nano-hybrid materials using nanoscale building blocks, (ii) the investigation of the interaction between light and nano-scale systems, (iii) the experimental study of the energy transfer and conversion in nanostructures down to single quantum dot / molecule level, and (iv) the development of novel experimental approaches to control, manipulate and probe with light on nanoscale.

HIGHLIGHT

Strong magneto-optical activity of an organic material coupled to plasmonic nanostructures. How to observe magnetic response from nonmagnetic materials

Melnikau D, Govyadinov AA, Sanchez-Iglesias A, Grzelczak M, Liz-Marzan LM, and Rakovich YP.

Nano Letters 17, 1808 (2017)

Plasmonic nanoparticles can significantly modify the optical properties of nearby organic molecules and thus present an attractive opportunity for sensing applications. In this paper, authors show that nonmagnetic organic molecules may exhibit magneto-optical response due to binding to a plasmonic nanoparticle.

Methods based on magneto-optical (MO) activity measurements, such as magnetic circular dichroism (MCD) spectroscopy and magneto-optic Kerr effect (MOKE), take an important place in the battery of tools for materials. However, direct MCD or MOKE measurements are rarely utilized in biosciences due to the usually very low magneto-optical response of biomolecules. Instead, magnetic methods for chemo- and biosensing typically rely on magneto-plasmonic effects, such as the high MO activity exhibited by plasmonic nanoparticles near their localized surface plasmon resonance. From other hand the utilization of plasmonic nanoarticles in sensing based on conventional absorption, fluorescence, or Raman spectroscopy techniques is often ineffective due to strong absorption background and light scattering, particularly in the case of turbid solutions, cell suspensions, and biological tissues.

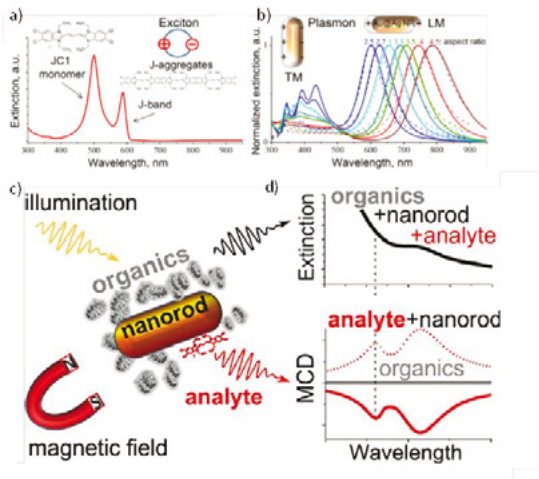


Figure 1: *Extinction spectra of the cyanine dye in J-aggregate state a) and bare core-shell Au@Ag nanorods of varying aspect ratios (solid lines), b) overlaid with theoretical predictions (dashed lines). Panels c) and d) show sketch of hybrid organic-inorganic system and corresponding extinction and MCD spectra.*

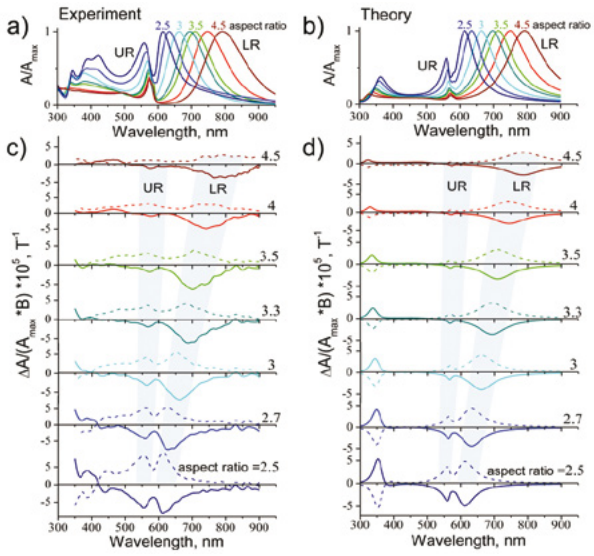


Figure 2: *Experimental a) and theoretical b) extinction spectra of the hybrid system of J-aggregates and core-shell Au@Ag nanorods for different aspect ratios. Experimental c) and theoretical d) MCD spectra measured under the applied magnetic fields of B =±1T.*

Recently we demonstrated that the MO activity of an organic compound itself can be greatly enhanced by coupling to a resonant plasmonic nanoparticle. Specifically, we show that supramolecular J-aggregates (a good model system for assemblies in biological complexes) linked to core-shell Au@Ag nanorods produce strong MCD signal when the resonance of the plasmonic nanoparticles is tuned to the excitonic band of the aggregates, while exhibiting no MCD upon detuning.

We explained such an enhancement of the MO activity by strong coupling of the J-band exciton and the nanoparticle plasmon and fully support our experimental findings by theoretical modelling. Strong-field confinement around the nanoparticle selectively enhances the MO activity only in those molecules that are bound to the particle surface. The near-complete absence of MO background from other molecular components could allow for the molecule detection even in the case of strong absorption background or light scattering. Thus, our work creates a new paradigm in sensing, which can make a large impact in materials science, medicine, biology, and pharmacology.

Group leader: Rolindes Balda de la Cruz, University Professor, UPV/EHU

13 Laser Physics and Photonic Materials

The activity of the "Laser Physics and Photonic Materials" group concentrates most of the research efforts on the study of optoelectronic properties of new materials and structures for solid state lasing and photonic crystal properties.

In recent years, the following specific objectives have been pursued on this topic: (i) the investigation on rare earth-doped vitroceramics for integrated optics applications, (ii) the study of the laser emission processes in dye-doped micro-nano structured hybrid materials for optoelectronic and biomedical applications, (iii) the synthesis and development of new eutectic materials for biomedical applications, (iv) the study of slow light in micro-nano structured materials with forbidden band gaps, (v) the experimental and theoretical study of the light generation in rare-earth doped micro-nano-crystalline dielectric powders for infrared random lasers, (vi) the study of laser-induced refrigeration in rare earth-doped micro-nano structured materials, and (vii) the design and making up of an optical wave guide writing system by using a femtosecond laser.

HIGHLIGHT

Oxyfluoride glass–ceramic fibers doped with Nd3+: structural and optical Characterisation

G. Gorni, R. Balda, J. Fernández, I. Iparraguirre, J. J. Velázquez, Y. Castro, L. Pascual, G. Chen, M. Sundararajan, M. J. Pascual, and A. Durán

CrystEngComm 19, 6620 (2017)

In the last few decades the growing interest in glass–ceramics (GCs), i.e. glasses that undergo controlled crystallization, has revealed the potential of this new class of optical materials, the properties of which, especially the optical ones, significantly improvred with controlled crystallization of certain crystalline phases.

Oxyfluoride glass–ceramics (OxFGCs) combining oxide matrices with low-phonon-energy fluoride crystals showed the possibility of increasing the optical efficiency of rare earth ions (REI), the most widely used active ions in the field of photonics, and at the same time of obtaining a strong material in terms of thermal, mechanical, and chemical resistances.

Most of the studies on OxFGCs doped with REI are about their optical properties as bulk materials and a few deal with thin films, but however, very few works have been published about OxFGC fibers.

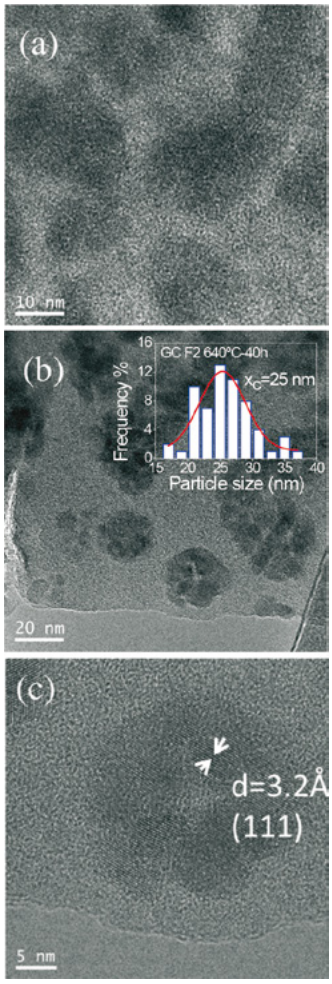


Figure 1: *HRTEM images of a) Glass fiber and b) GC fiber treated at 640 °C–40 h. The phase separation droplets are clearly visible with an average size of around 25 nm. The crystal segregation inside the droplets is likely due to residual Si and Al diffusion that forms very thin shells of high viscosity. c) Details of a phase separation droplet with LaF3 crystals inside. The interplanar distance obtained is 3.2 Å, attributed to (111) planes of the hexagonal LaF3 crystalline phase.*

In this collaborative work carried out by the groups led by Alicia Durán (ICV, CSIC) and Rolindes Balda (CFM, UPV/EHU), transparent OxFGC optical fibers doped with Nd3+ were successfully prepared by a single crucible method, then heat treated to convert them into GC and finally covered with SiO2 cladding using the sol–gel method. A detailed structural Characterisation performed by XRD, HRTEM and SAXS showed that phase separation in the as made glass fibers is precursor for crystallization and also that the crystallization mechanism is a diffusion-controlled process that limits the precipitation of LaF3 nano-crystals (NCs) to a size of 9-15 nm.

The optical Characterisation demonstrated the light propagation into the glass–ceramic core and the possibility to selectively excite Nd3+ ions in the fluoride nanocrystals with a corresponding increase of the luminescence efficiency. Site-selective emission and excitation laser spectroscopy allows isolation of the emission of Nd3+ ions in LaF3 NCs and thus reproduction of the same luminescence properties of pure Nd3+ doped LaF3 crystals. It is worth noting that these oxyfluoride glass fibers present the great advantage of maintaining the precursor crystalline phase during the drawing process, which allows thermal control of the size of the crystallites in the resulting glass–ceramic fibers as well as preservation of their optical guidance.

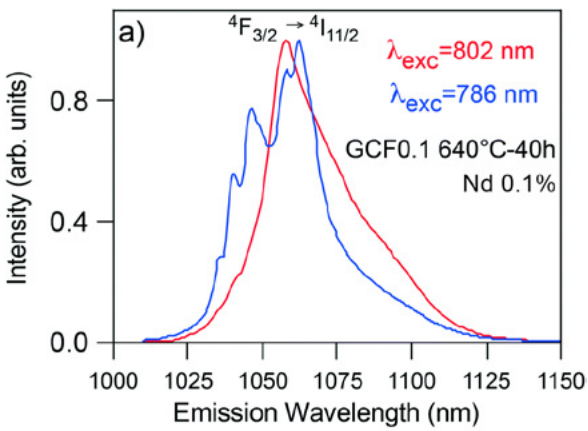


Figure 2: *Normalized emission spectra obtained under excitation at 786 and 802 nm for the GC fiber doped with 0.1 mol% NdF3. The spectrum obtained under excitation at 786 nm corresponds to Nd3+ ions in the LaF3 NCs, whereas the one obtained under excitation at 802 nm shows an inhomogeneously broadened band similar to that of the glass sample.*

Group leader: Gabriel Molina Terriza, Ikerbasque Professor, MPC

14

Quantum Nanophotonics Laboratory

Gabriel Molina Terriza, a former Professor at Macquarie University in Sidney, has joined CFM in 2017. Prof. Molina Terriza develops research on Quantum Information with entangled Photons, and has joined CFM to launch a new experimental group on Quantum Nanophotonics. This strategic decision puts the CFM in a privileged situation to face opportunities arising from the European flagship on "Quantum Technologies" to be launched in Europe.

The Centre for Materials Physics seeks to exploit the potential and expertise of the theory groups on quantum states, and complement it with the experimental effort by this new group that can approach this topic from an applied and technological point of view. Professor Gabriel Molina Terriza will be responsible for launching and designing the objectives on this topic in the centre during the next years.

The research program of the "Quantum Nanophotonics Laboratory" group aims at contributing to the development of hybrid quantum devices based on the interaction of light and matter at the nanoscale.

POLYMERS AND SOFT MATTER

15

Polymers and Soft Matter

The research activity of the "Polymers and Soft Matter" group deals with the experimental and theoretical study of polymers and soft condensed matter. This activity mainly focuses on the investigation of the structure and dynamics of polymers and glass-forming complex systems (multi-component, nano-structured and biopolymer materials), in general, at different length and time scales (micro, nano, meso, macro). The methodological approach developed at CFM to tackle this research line is based on a combination of relaxation techniques, neutron and X-ray scattering, microscopy techniques and molecular dynamics simulations. A combination of experimental, theoretical and simulation efforts, together with the development of advanced chemical synthesis routes, is essential to progress in this interdisciplinary area.

A group of nine tenured scientists belonging to CSIC, UPV/EHU and Ikerbasque develop the different aspects of this research line.

In recent years, the following specific objectives have been targeted in this research activity: (i) understanding of the interplay of geometry and topology in polymeric materials, (ii) the characterisation of interfacial features, and (iii) the study of the dynamics at the interfacial level, the new confinement effects and the way local friction arises in crowed environments. The experimental effort that covers these objectives is developed in a set of laboratories in the centre that are equipped with a variety of microscopy and spectroscopy techniques. Among others, a Scanning Electron Microscope,

dielectric spectrometers and a spectrometer of low-angle X-ray diffraction are located in the centre and are run by one of the members of the research group, giving service to the research community. This group shows a strong connection with private companies, which hire the services of the group to study and characterise particular forms of soft matter, such as rubber.

HIGHLIGHT 1

Reaching the ideal glass transition by aging polymer films

Boucher VM, Cangialosi D, Alegria A, and Colmenero J.

Physical Chemistry Chemical Physics 19, 961 (2017)

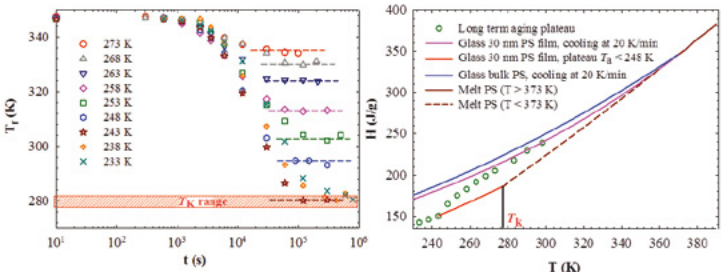
We exploited the ability of glasses with large amount of free interfacial area to access low energy state in remarkably short times scale. To this aim, we employed thin polymer films and study how equilibrium is recovered deep in the glassy state. We showed how these systems are able to access a thermodynamic state, the ideal glass, with the entropy of the crystal.

A system out of thermodynamic equilibrium spontaneously tends to decrease its free energy. Glasses belong to the category of nonequilibrium systems. In this case, the closest accessible free energy minima are the equilibrium supercooled liquid and the crystalline state. Evolution toward the thermodynamic state of the supercooled liquid is generally addressed as "physical aging". In bulk glass-formers, accessing such state requires experimentally unfeasible time scales already at temperatures close to the glass transition temperature (Tg). This has so far left unsolved one of the most important aspects of glass thermodynamics, originating from the observation that, if the entropy of the supercooled liquid is extrapolated below Tg, there will be a temperature, so-called Kauzmann temperature (TK), at which the entropy of such disordered liquid would equal that of the ordered crystal. This paradoxical scenario implies the violation of the third principle of thermodynamics, given the fact that at lower temperatures the entropy of the liquid would become lower than that of the crystal. A true thermodynamic transition, the ideal glass transition, is hypothesized to overcome the entropy catastrophe.

Thus, we exploited the ability of thin polymer films to equilibrate over considerably shorter time scales than the bulk. In other words, in films there exists an alternative pathway toward equilibrium. To this aim, the time evolution of the enthalpy occurring during physical aging of 30 nm thick PS films was investigated. This system exhibits two mechanisms of equilibration, similarly to bulk PS. The "fast" mechanism allows massive enthalpy recovery toward equilibrium, as testified by the considerable decrease of the fictive temperature (Tf). This quantifies how low in the energy the glass is and is defined as the temperature a glass with given thermodynamic state would be at equilibrium (see Figure, left panel). Notably this occurs in time scales shorter than several days. When aged far below Tg, these films are

able to access a thermodynamic state with entropy equal to that of the crystal (see Figure, right panel). The most important consequence of this finding is that the thermodynamic (ideal) glass transition does actually exist at TK.

Figure: *(Left panel) aging time evolution of fictive temperature in 30 nm thick stacked PS films at the indicated temperatures; (Right panel) enthalpy plot showing the thermodynamic state achieved by such films in the indicated conditions.*



HIGHLIGHT 2

The role of the topological constraints in the chain dynamics in all polymer nanocomposites

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

Macromolecules 50, 1719 (2017)

In a long-lasting effort to get a good compatibility between the nanoparticles and the linear polymer matrix, all-polymer nanocomposites are gaining increasing attention. The presence of soft penetrable polymer nanoparticles in such systems is expected to affect the fundamental topological constraints (entanglements) that originate from chain uncrossability and that control the viscoelastic properties of the system. In this pioneering computational study of all-polymer nanocomposites, the authors shed light on this question by discussing simulations in the framework of the tube model.

They investigate all-polymer nanocomposites, formed by strongly entangled linear chains and single-chain polymer nanoparticles (SCNPs), by means of large-scale simulations. SCNPs are soft nano-objetcs obtained through intramolecular cross-linking of linear chains, with potential applications as nanocarriers, catalytic or rheological agents, among others. To distinguish the role of the soft penetrable character of the SCNPs in the topological constraints from other specific contributions present in experiments, the simulations are performed at constant density and with identical segmental mobility and monomer excluded volume for the SCNPs and the linear chains. Every composition leads to a well-dispersed nanocomposite with fully penetrated nanofillers. Hence, unlike in the case of composites with hard nanofillers, the SCNPs do not exert confinement effects on the linear chains and only contribute to the topological constraints.

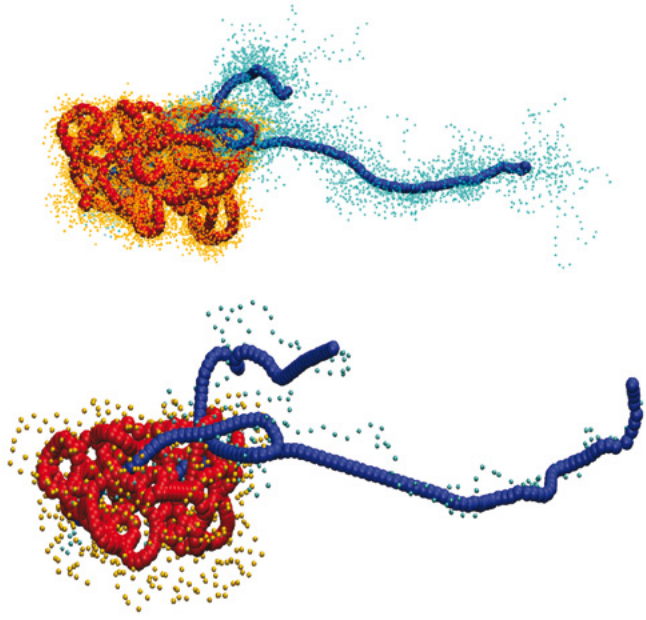


Figure: *IMP and PP of a globular SCNP and a penetrating linear chain. The coordinates of the red (SCNP) and blue (chain) monomers are obtained after applying the IMP procedure (top panel) and the PP construction (bottom panel). The coordinates of the real configurations used for such constructions are drawn as yellow (SCNP) and cyan dots (chain).*

The intramolecular dynamics of the linear chains in terms of the tube model are discussed. The authors determine the entanglement length of the linear chains by analysing their isoconfigurational mean paths (IMP) and the primitive paths (PP) (see figure) as a function of the concentration and topology of the SCNPs. In the analysis we use different estimators proposed in the literature. The IMP and PP analysis in the nanocomposites with sparse SCNPs yields values of the entanglement length smaller and larger, respectively, than in the reference pure linear melt, though small variations are observed. A more consistent trend is found in the nanocomposites with globular SCNPs, where both the IMP and PP analysis unambiguously reveal that the linear chains are more entangled than in the pure linear melt ("tube narrowing"). Such differences between the effects of SCNPs with different topologies are presumably related to the much higher fraction of threadable loops present in the globular SCNPs, with respect to their sparse counterparts, which effectively lead to more topological constraints.

The optical Characterisation demonstrated the light propagation into the glass–ceramic core and the possibility to selectively excite Nd3+ ions in the fluoride nanocrystals with a corresponding increase of the luminescence efficiency. Site-selective emission and excitation laser spectroscopy allows isolation of the emission of Nd3+ ions in LaF3 NCs and thus reproduction of the same luminescence properties of pure Nd3+ doped LaF3 crystals. It is worth noting that these oxyfluoride glass fibers present the great advantage of maintaining the precursor crystalline phase during the drawing process, which allows thermal control of the size of the crystallites in the resulting glass–ceramic fibers as well as preservation of their optical guidance.

FACILITIES & EXTERNAL SERVICES

CFM infrastructure has been envisioned to characterise nanoscale materials with high sensitivity. Thus, CFM headquarters building was built on the basis of sophisticated architectural and engineering solutions to create a unique environment, free of electromagnetic interference and with an ultralow level of vibration. Since the opening of CFM headquarters in 2010, state-of-the-art facilities have been launched progressively, which complete a set of very sophisticated and specialised experimental techniques, ready to give response to the needs in advanced materials characterisation. These needs involve both fundamental research in nanomaterials, as well as specifically targeted systems of interest for energy and in bio-environmental strategic areas. The following equipment and infrastructures are hosted and run at CFM by the different research groups:

FACILITIES

HIGH RESOLUTION ANGLE RESOLVED PHOTOEMISSION LAB

The “High Resolution Angle Resolved Photoemission” laboratory is equipped with an Angle Resolved Photoemission Spectroscopy (ARPES) system combined with atomic-resolved microscopy (Scanning Tunnel Microscope, STM). These two techniques can be used either jointly or separately. The ARPES instrument allows achieving ultra-high resolution (0.1 degrees, 5 meV) and can deal with samples at low temperature (20K).

DIELECTRIC SPECTROSCOPY LAB

The “Dielectric Spectroscopy” laboratory provides characterisation of dielectric properties of polymer and soft matter samples. The combined use of several types of spectrometers, listed below, allows covering a wide dynamical range of more than 16 orders of magnitude (in frequency and time domain) and different sample environments:

- Broad-Band Dielectric Spectrometers (BBDS): ALPHA-S & ALPHA-A Novocontrol
- High-Frequency Dielectric Spectrometer (HFDS): Agilent E4991A RF-Impedance Analyzer
- Micro-Wave Dielectric Spectrometer (MWDS): Agilent E8361A Microwave Network Analyzer
- Therahertz Spectrometer (THS): Teraview 3000 spectrometer
- High-Pressure Dielectric Spectrometer (HPDS): Concept 100 Novocontrol
- Low-Temperature Dielectric spectrometer (LTDS): ALPHA-A Novocontrol
- Time-Domain Dielectric Spectrometer (TDDS): Novocontrol
- Thermally Stimulated Depolarization Currents (TSDC): Novocontrol

LASER SPECTROSCOPY LAB

In the “Laser Spectroscopy” laboratory, continuous and time-resolved (with nano-pico excitation laser sources) spectroscopies with high spectral resolution in the ultraviolet-visible-infrared (UV-VIS-IR) radiation domains, together with low temperature facilities (2K) are used to characterise the properties of rare-earth materias for lasing. A home-made photoacoustic spectrometer is also available. These facilities are physically located at the Engineering School of Bilbao (out of the CFM main premises in Donostia-San Sebastián).

ULTRAFAST SPECTROSCOPY LAB

The “Ultrafast Spectroscopy” laboratory consists of tunable femtosecond sources (with regenerative amplification) in the IR domain with high speed detectors in the picosecond domain (Streak camera), capable of measuring the fluorescence of atoms and ions of technological interest. There is also a multiphoton microscope with time-resolved possibilities to this end. These facilities are physically located at the Engineering School in Bilbao (out of the CFM main premises in Donostia-San Sebastián).

SURFACE CHEMISTRY LAB

The “Surface Chemistry” laboratory is equipped with techniques that provide samples surface characterisation by means of X Ray Photoemission (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), Atomic Force Microscope (AFM) and Scanning Tunnel Microscope (STM) (either combined or separately), with the required molecular beam epitaxy (MBE) and sample preparation.

FACILITIES

SURFACE MAGNETISM LAB

The “Surface Chemistry” laboratory hosts equipment for surface characterisation of samples by means of a home-made Magneto Optic Kerr Effect (MOKE, 77 800 K, 0.1 Tesla) and Scanning Tunnel Microscope (STM, Omicron, 70 800K) (combined or separately). The measuring ultra-high vacuum chamber includes Low Energy Electron Diffraction (LEED) and molecular beam epitaxy (MBE).

MICROSCOPY LAB

The “Microscopy” laboratory can characterise polymer and soft matter samples by means of:

- Optical Confocal Microscopy (Leica TCS SPE DM5500, 120 - 520K)
- Scanning Electron Microscopy (SEM, Hitachi TM 3000, 250 - 320 K)
- Atomic Force Microscopy (AFM, MultiMode V, Veeco, 250 - 470 K)

ULTRA-LOW TEMPERATURE SCANNING TUNNELING MICROSCOPY LAB

The “Ultra-Low Temperature Scanning Tunneling Microscopy” laboratory hosts an Atomic Force Microscopy (AFM)/ Scanning Tunnel Microscope (STM) that tunnels current at 1K for characterisation of materials at atomic scale.

NANOPHOTONICS LAB

The “Nanophotonics” laboratory hosts a scanning confocal time-resolved photoluminescence (TRPL) setup (MicroTime200, PicoQuant) providing single molecule sensitivity and high temporal resolution to measure the decay of quantum dot and molecular emitters. The range of application includes Fluorescence Lifetime Imaging (FLIM), Fluorescence Correlation Spectroscopy (FCS), Forster Resonance Energy Transfer (FRET), Fluorescence Lifetime Measurements, and Fluorescence Anisotropy and Intensity Time Traces.

CHEMISTRY LAB

The “Chemistry” laboratory is specialised in synthesis of polymer- and soft-matter based materials, with special focus on nanoparticles and click chemistry. This laboratory can characterise physicochemical properties and stability of supramolecular chemical compounds using the following equipment:

- Absolute molecular mass distribution meter: Agilent 1200 GPC-SEC Analysis System + Wyatt. Ligth-scattering miniDAWN TREOS and OptilabÂ rEX Refractive Index Detector
- Nanoparticle size and z-potential meter: Malvern Zetasizer Nano
- Viscometer: Malvern SV-10 Vibro
- Surface tension meter: Contact Angle meter OCA 15 EC DataPhysics Instruments GmbH
- Liquid/solution density meter: ANTON PAAR, DMA 4500 M model
- UV-VIS spectrometer: Agilent 8453A with Peltier thermostated cell holder, T-controller 89090A
- Close vessel microwave assisted reactor: CEM Discover SP System (200- 550 K, 0-27 bar)

X-RAY LAB

The “X-Ray” laboratory can provide characterisation of polymer and soft matter samples by means of the following techniques:

- Small Angle X-Ray Scattering (SAXS): Rigaku PSAXS-L (120 - 520 K) with simultaneous WASX measurements. This equipment is run by a technician with specific training
- Wide Angle X-Ray Scattering (WASX): Bruker AXS D8 ADVANCE (120 - 520 K)

MATERIALS SYNTHESIS LAB

In the “Materials Synthesis” laboratory, materials crystal growth is investigated by using home-made Bridgman and Czochralski fournaces.

FACILITIES

THERMAL ANALYSIS LAB

The “Thermal Analysis” laboratory hosts the following equipment to characterise polymer and soft matter samples:

- Differential Scanning Calorimetry analysis (DSC): Q2000 TMDSC - TA Instruments (100 - 700 K) and Flash DSC1 - Mettler Toledo (180 - 700 K)
- Thermogravimetric analysis (TGA): Q500, TA Instruments (290 - 1300 K)
- Dilatometry (DIL): Zero Friction L75V, Linseis (100 - 800 K) dual push rod version
- Pressure-Volume-Temperature (PVT): PVT100, Thermo Haake (200 - 550 K, 200 - 2500 Bar)

MECHANICAL CHARACTERISATION LAB

The “Mechanical characterisation” laboratory hosts the following equipment to perform rheological analysis in polymer and soft matter samples:

- ARES-LS2 rheometer - TA Instruments (130 - 800 K) (1mHz - 50 Hz), with simultaneous electric impedance analyser (20Hz - 1MHz)
- Minimat 200 Rheometrics Scientific (200 - 500 K) miniature material tester

MOLECULAR SPECTROSCOPY LAB

The “Molecular Spectroscopy” laboratory hosts the following equipment to characterise polymer and soft matter samples by means of molecular spectroscopy:

- For the molecular spectroscopy in the infrared (IR) domain: FT-IR - JASCO 6300 (130 - 400 K)
- For the molecular spectroscopy in the terahertz (THz) domain: TPS SPECTRA 3000, TeraView

SPECTROSCOPY TECHNIQUES LAB

In the “Spectroscopy Techniques” laboratory, a Varian Cary50 spectroscopic equipment is used to investigate materials energy transfer and conversion.

HIGH PERFORMANCE COMPUTING (HPC) CENTRE

The “Computing Centre” consists of two High Performance Computing (HPC) clusters:

- Oberon cluster (the main CFM HPC cluster) is composed of 174 computing nodes with two Xeon processors and at least 24GB of memory on each node, all of them sharing a high speed-low latency Infiniband connection network, giving a total of around 1936 cores and ~5TB of memory.
- Nostromo cluster is designed for shared memory – single node calculations. It is composed of 17 AMD Opteron 6300 series computing nodes with 64 cores and 64GB of RAM each node, giving a total of 1088 cores and about 1TB of memory.

These two clusters give service to a variety of computational needs in the centre, mainly to the ab-initio calculation of advanced materials, which is a transverse topic within the centre. Apart from these clusters, there are 11 workstations in order to run specific numerical applications.

EXTERNAL SERVICES

CFM offers external services based on the centre equipment and infrastructure to academic and industrial users. External services are open facilities carried out by CFM qualified researchers and technicians for researchers and technologists from different research fields and businesses. The CFM external services that can be commissioned are as follows:

DIELECTRIC SPECTROSCOPY LAB

- Characterisation of dielectric properties of polymer and soft matter samples

SURFACE CHEMISTRY LAB

- Materials surface characterisation by means of X-ray Photoelectron Spectroscopy, Ultraviolet Photoemission Spectroscopy, Atomic Force Microscopy and Scanning Tunnel microscopy, XPS/UPS/AFM/STM (either combined of separately)

MICROSCOPY LAB

- Characterisation of materials microstructure by means of Scanning Electron Microscopy (SEM)
- Characterisation of polymer and soft matter samples by means of Atomic Force Microscopy (AFM)

NANOPHOTONICS LAB

- Time-resolved photoluminescence (TRPL) measurements

CHEMISTRY LAB

- Characterisation of physicochemical properties and stability of supramolecular chemical compounds

X-RAY LAB

- Characterisation of polymer and soft matter samples by means of Small Angle X-Ray Scattering (SAXS) and Wide Angle X-Ray Diffractometer (WASX) techniques

THERMAL ANALYSIS LAB

- Characterisation of polymer and soft matter samples by means of Differential Scanning Calorimetry (DSC) and Thermogravimetry (TG) techniques
- Determination of Linear Thermal expansion coefficients of polymer and soft matter samples by means of dilatometry and Pressure Volume Temperature (PVT) analysis

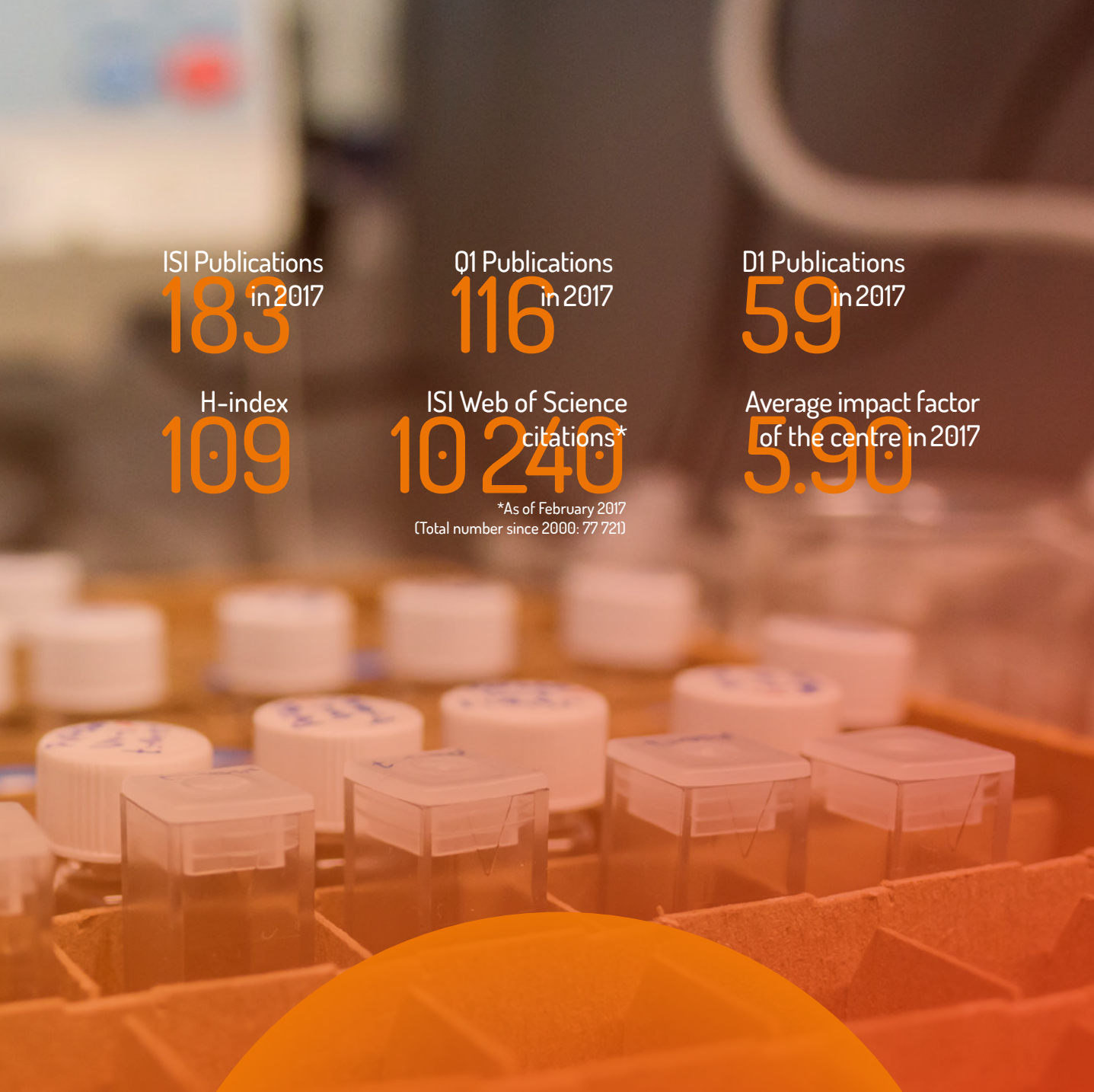
MOLECULAR SPECTROSCOPY LAB

- Molecular characterisation of polymer and soft matter samples by means of spectroscopy in the infrared (IR) and terahertz (THz) domains

HIGH PERFORMANCE COMPUTING (HPC) CENTRE

- Technical support and consulting service for the design, implementation, installation and optimization of software for HPC applications
- Technical support and scientific consulting service for modelling, computing and simulation in the domain of Materials Sciences (electronic structure techniques, classical and semiclassical models, molecular dynamics, Monte-Carlo, etc.)

RESEARCH OUTPUT



ISI Publications in 2017
183

Q1 Publications in 2017
116

D1 Publications in 2017
59

H-index
109

ISI Web of Science citations*
10 240

*As of February 2017
(Total number since 2000: 77 721)

Average impact factor of the centre in 2017
5.90

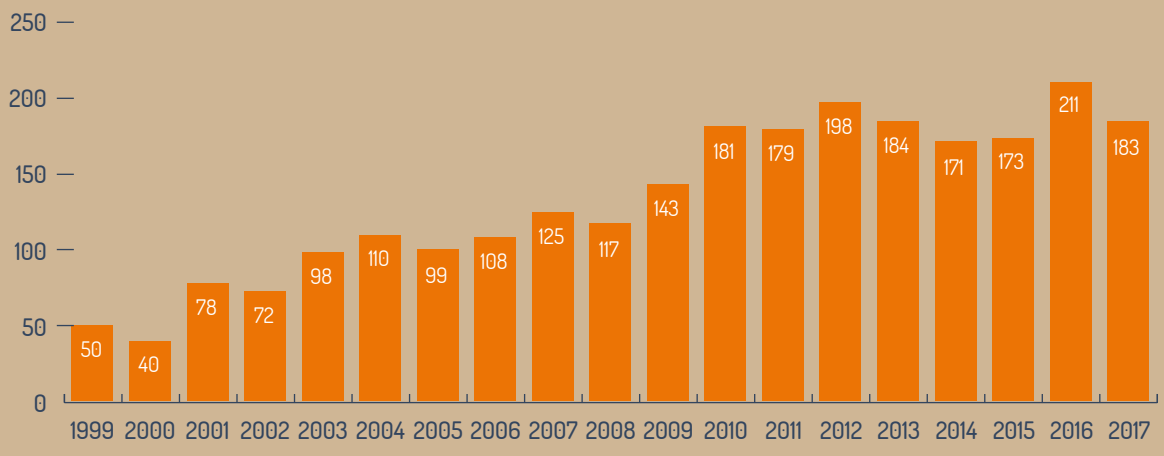
Among all the articles published at CFM, **81 %** (149 out of 181) were published in the framework of **international collaborations,** showing the international dimension and positioning of the Centre in the field of Materials Science.

6% of the internationally co-authored papers were published in collaboration with groups belonging to five of the top-ten universities worldwide, according to the Shanghai Academic Ranking of World Universities (ARWU) in Natural Science and Mathematics (SCI) for 2016. These six universities are: University of California Berkeley, Stanford University, Massachusetts Institute of Technology (MIT), University of Cambridge and University of Tokyo.

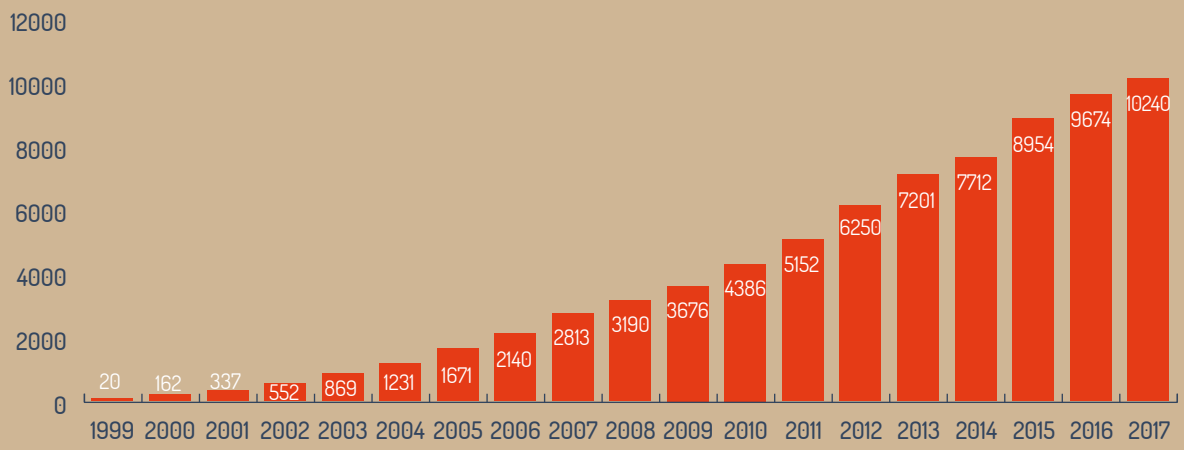
RESEARCH OUTPUT

	2010	2011	2012	2013	2014	2015	2016	**2017**
ISI PUBLICATIONS	181	179	198	184	171	173	211	**183**
Q1	134	144	149	139	131	129	178	**116**
D1	-	-	-	-	52	50	74	**59**

PUBLICATIONS



CITATIONS



*Source Web of Science Core Collection - CFM's Researcher ID: F-4867-2012

Total number of publications in and above Nano Research

Journal	Number of articles	Impact factor
Nature Materials	1	39.73
Chemical Society Reviews	1	38.62
Science	1	37.20
ACS Nano	8	13.94
Nano Letters	7	12.71
Nature Communications	8	12.12
Angewandte Chemie-International	1	11.99
ACS Catalysis	1	10.61
Chemistry Of Materials	2	9.47
Journal Of Physical Chemistry Letters	1	9.35
Progress in Surface Science	2	8.62
Physical Review Letters	4	8.46
Laser Photonics Reviews	1	8.43
Nanoscale	4	7.37
Nano Research	1	7.35

PUBLICATIONS

1 **Electronics and optoelectronics of quasi-1D layered transition metal trichalcogenides**
Island JO, Molina-Mendoza AJ, Barawi M, Biele R, Flores E, Clamagirand JM, Ares JR, Sanchez C, van der Zant HSJ, D'Agosta R, Ferrer IJ, and Castellanos-Gomez A.
2D Materials 4, 022003 (2017)

2 **Highly-ordered wide bandgap materials for quantized anomalous Hall and magnetoelectric effects**
Otrokov MM, Menshchikova TV, Vergniory MG, Rusinov IP, Vyazovskaya AY, Koroteev YM, Bihlmayer G, Ernst A, Echenique PM, Arnau A, and Chulkov EV.
2D Materials 4, 025082 (2017)

3 **Square selenene and tellurene: novel group VI elemental 2D materials with nontrivial topological properties**
Xian LD, Paz AP, Bianco E, Ajayan PM, and Rubio A.
2D Materials 4, 041003 (2017)

4 **Tuning the Graphene on Ir(111) adsorption regime by Fe/Ir surface-alloying**
Brede J, Slawinska J, Abadia M, Rogero C, Ortega JE, Piquero-Zulaica I, Lobo-Checa J, Arnau A, and Cerda JI.
2D Materials 4, 16 (2017)

5 **Strain Dependent Light-off Temperature in Catalysis Revealed by Planar Laser-Induced Fluorescence**
Blomberg S, Zetterberg J, Zhou JF, Merte LR, Gustafson J, Shipilin M, Trinchero A, Miccio LA, Magana A, Ilyn M, Schiller F, Ortega JE, Bertram F, Gronbeck H, and Lundgren E.
ACS Catalysis 7, 110 (2017)

6 **Irreversible Adsorption Erases the Free Surface Effect on the T-g of Supported Films of Poly(4-tert-butylstyrene)**
Perez-de-Eulate NG, Sferrazza M, Cangialosi D, and Napolitano S.
ACS Macro Letters 6, 354 (2017)

7 **Glass Transition and Molecular Dynamics in Polystyrene Nanospheres by Fast Scanning Calorimetry**
Perez-de-Eulate NG, Di Lisio V, and Cangialosi D.
ACS Macro Letters 6, 859 (2017)

8 **Reply to - Comment on 'Spin-Orbit Coupling Induced Gap in Graphene on Pt(111) with Intercalated Pb Monolayer**
Klimovskikh II, Otrokov MM, Voroshnin VY, Sostina D, Petaccia L, Di Santo G, Thakur S, Chulkov EV, and Shikin AM.
ACS Nano 11, 10630 (2017)

9 **Width-Dependent Band Gap in Armchair Graphene Nanoribbons Reveals Fermi Level Pinning on Au(111)**
Merino-Diez N, Garcia-Lekue A, Carbonell-Sanroma E, Li JC, Corso M, Colazzo L, Sedona F, Sanchez-Portal D, Pascual JI, and de Oteyza DG.
ACS Nano 11, 11661 (2017)

10 **Polymerization of Well-Aligned Organic Nanowires on a Ferromagnetic Rare-Earth Surface Alloy**
Abadia M, Ilyn M, Piquero-Zulaica I, Gargiani P, Rogero C, Ortega JE, and Brede J.
ACS Nano 11, 12392 (2017)

PUBLICATIONS

11 **Spin-Orbit Coupling Induced Gap in Graphene on Pt(111) with Intercalated Pb Monolayer**
Klimovskikh II, Otrokov MM, Voroshnin VY, Sostina D, Petaccia L, Di Santo G, Thakur S, Chulkov EV, and Shikin AM.
ACS Nano 11, 368 (2017)

12 **Electric-Field-Driven Direct Desulfurization**
Borca B, Michnowicz T, Petuya R, Pristl M, Schendel V, Pentegov I, Kraft U, Klauk H, Wahl P, Gutzler R, Arnau A, Schlickum U, and Kern K.
ACS Nano 11, 4703 (2017)

13 **Raman Spectroscopy of Lattice-Matched Graphene on Strongly Interacting Metal Surfaces**
Usachov DY, Davydov VY, Levitskii VS, Shevelev VO, Marchenko D, Senkovskiy BV, Vilkov OY, Rybkin AG, Yashina LV, Chulkov EV, Sklyadneva IY, Heid R, Bohnen KP, Laubschat C, and Vyalikh DV.
ACS Nano 11, 6336 (2017)

14 **Doping of Graphene Nanoribbons via Functional Group Edge Modification**
Carbonell-Sanroma E, Hieulle J, Vilas-Varela M, Brandimarte P, Lraola M, Barragan A, Li JC, Abadia M, Corso M, Sanchez-Portal D, Pena D, and Pascual JI
ACS Nano 11, 7355 (2017)

15 **On-Surface Oligomerization of Self Terminating Molecular Chains for the Design of Spintronic Devices**
Sierda E, Abadia M, Brede J, Elsebach M, Bugenhagen B, Prosenc MH, Bazarnik M, and Wiesendanger R.
ACS Nano 11, 9200 (2017)

16 **Optical Polarization Mobius Strips on All-Dielectric Optical Scatterers**
Garcia-Etxarri A.
ACS Photonics 4, 1159 (2017)

17 **Enhancing Enantioselective Absorption Using Dielectric Nanospheres**
Ho CS, Garcia-Etxarri A, Zhao Y, and Dionne J.
ACS Photonics 4, 197 (2017)

18 **Electric Field-Induced High Order Nonlinearity in Plasmonic Nanoparticles Retrieved with Time-Dependent** Density Functional Theory
Aguirregabiria G, Marinica DC, Esteban R, Kaiansky AK, Aizpurua J, and Borisov AG.
ACS Photonics 4, 613 (2017)

19 **Reversible and Irreversible Reactions of Trimethylaluminum with Common Organic Functional Groups as a Model for Molecular Layer Deposition and Vapor Phase Infiltration**
Yang F, Brede J, Ablat H, Abadia M, Zhang LB, Rogero C, Elliott SD, and Knez M.
Advanced Materials Interfaces 4, 1700237 (2017)

20 **MoS2-Carbon Nanotube Hybrid Material Growth and Gas Sensing**
Deokar G, Vancso P, Arenal R, Ravaux F, Casanova-Chafer J, Llobet E, Makarova A, Vyalikh D, Struzzi C, Lambin P, Jouiad M, and Colomer JF.
Advanced Materials Interfaces 4, 1700801 (2017)

PUBLICATIONS

21 **Nanoscale Chemical Imaging of Interfacial Monolayers by Tip-Enhanced Raman Spectroscopy**
Shao F, Muller V, Zhang Y, Schluter AD, and Zenobi R
Angewandte Chemie- International Edition 56, 9361 (2017)

22 **Structural Characterisation of a Covalent Monolayer Sheet Obtained by Two-Dimensional Polymerization at an Air/Water Interface**
Muller V, Shao F, Baljozovic M, Moradi M, Zhang Y, Jung T, Thompson WB, King BT, Zenobi R, and Schluter AD.
Angewndte Chemie- International Edition 56, 15262 (2017)

23 **Temperature dependence of the partially localized state in a 2D molecular nanoporous network**
Piquero-Zulaica I, Nowakowska S, Ortega JE, Stohr M, Gade LH, Jung TA, and Lobo-Checa J.
Applied Surface Science 391, 39 (2017)

24 **Formation of polymer nanoparticles by UV pulsed laser ablation of poly (bisphenol A carbonate) in liquid environment**
Martinez-Tong DE, Sanz M, Ezquerra TA, Nogales A, Marco JF, Castillejo M, and Rebollar E.
Applied Surface Science 418, 522 (2017)

25 **Effect of the fluorination technique on the surface-fluorination patterning of double-walled carbon nanotubes**
Bulusheva LG, Fedoseeva YV, Flahaut E, Rio J, Ewels CP, Koroteev VO, Van Lier G, Vyalikh DV, and Okotrub AV.
Beillstein Journal of Nanotechnology 8, 1688 (2017)

26 **Magnetic coupling between 3d transition metal adatoms on graphene supported by metallic substrates**
Petuya R, and Arnau A.
Carbon 116, 599 (2017)

27 **Experimental and theoretical high pressure study of calcium hydroxyaluminate phases**
Cuesta A, Rejmak P, Ayuela A, De la Torre AG, Santacruz I, Carrasco LF, Popescu C, and Aranda MAG.
Cement and Concrete Research 97, 1 (2017)

28 **Mastering high resolution tip-enhanced Raman spectroscopy: towards a shift of perception**
Richard-Lacroix M, Zhang Y, Dong ZC, and Deckert V.l
Chemical Society Reviews 46, 3922 (2017)

29 **Modular Design with 2D Topological-Insulator Building Blocks: Optimized Synthesis and Crystal Growth and Crystal and Electronic Structures of BixTeI (x=2, 3)**
Zeugner A, Kaiser M, Schmidt P, Menshchikova TV, Rusinov IP, Markelov AV, Van den Broek W, Chulkov EV, Doert T, Ruck M, and Isaeva A.
Chemistry of materials 29, 1321 (2017)

30 **Relaxations and Relaxor-Ferroelectric-Like Response of Nanotubularly Confined Poly(vinylidene fluoride)**
Martin J, Iturrospe A, Cavallaro A, Arbe A, Stingelin N, Ezquerra TA, Mijangos C, and Nogales A.
Chemistry of Materials 29, 3515 (2017)

31 **Comparison of performance of van der Waals-corrected exchange-correlation functionals for interlayer interaction in graphene and hexagonal boron nitride**
Lebedeva IV, Lebedev AV, Popov AM, and Knizhnik AA.
Computational Material Science 128, 45-58 (2017)

PUBLICATIONS

32 **Improvements on non-equilibrium and transport Green function techniques: The next-generation TRANSIESTA**
Papior N, Lorente N, Frederiksen T, Garcia A, and Brandbyge M.
Computer Physics Communications 212, 8 (2017)

33 **Reversible Thermosalient Effect of N'-2-Propylidene-4-hydroxybenzohydrazide Accompanied by an Immense Negative Compressibility: Structural and Theoretical Arguments Aiming toward the Elucidation of Jumping Phenomenon**
Loncaric I, Popovic, J, Despoja V, Burazer S, Grgicevic I, Popovic D, and Skoko Z.
Crystal Growth & Design 17, 4445 (2017)

34 **Capsulate structure effect on SWNTs doping in RbxAg1-xI@SWNT composites**
Falaleev NS, Kumskov AS, Zhigalina VG, Verbitskiy II, Vasiliev AL, Makarova AA, Vyalikh DV, Kiselev NA, and Eliseev AA.
Crystengcomm 19, 3063 (2017)

35 **Oxyfluoride glass-ceramic fibers doped with Nd3+: structural and optical Characterisation**
Gorni G, Balda R, Fernandez J, Iparraguirre I, Velazquez JJ, Castro Y, Pascual L, Chen G, Sundararajan M, Pascual MJ, and Duran A.
Crystengcomm 19, 6620 (2017)

36 **Review-Towards the Next Generation of Thermoelectric Materials: Tailoring Electronic and Phononic Properties of Nanomaterials**
Caballero-Calero O, and D'Agosta R.
ECS Journal of Solid State Science and Technology 6, N3065 (2017)

37 **Efficient and accurate modeling of electron photoemission in nanostructures with TDDFT**
Wopperer P, De Giovannini U, and Rubio A.
European Physical Journal B 90, 51 (2017)

38 **Poly(butylene succinate-ran-epsilon-caprolactone) copolyesters: Enzymatic synthesis and crystalline isodimorphic character**
Ciulik C, Safari M, de Ilarduya AM, Morales-Huerta JC, Iturrospe A, Arbe A, Muller AJ, and Munoz-Guerra S.
European Polymer Journal 95, 795 (2017)

39 **Theory of SERS enhancement: general discussion**
Graham D, Goodacre R, Arnolds H, Masson JF, Schatz G, Baumberg J, Kim DH, Aizpurua J, Lum W, Silvestri A, de Nijs B, Xu YK, Di Martino G, Natan M, Schlucker S, Wuytens P, Bruzas I, Kuttner C, Hardy M, Chikkaraddy R, Sabanes NM, Delfino I, Dawson P, Gawinkowski S, Bontempi N, Mahajan S, Reich S, Hourahine B, Bell S, Krolikowska A, Porter M, Keeler A, Kamp M, Fountain A, Fasolato C, Giorgis F, Otero JC, Matricardi C, Van Duyne R, Lombardi J, Deckert V, and Velleman L.
Faraday Discussions 205, 173 (2017)

40 **Ultrasensitive and towards single molecule SERS: general discussion**
Aizpurua J, Arnolds H, Baumberg J, Bruzas I, Chikkaraddy R, Chisanga M, Dawson P, Deckert V, Delfino I, de Nijs B, Di Martino G, Edel J, Fleming H, Gawinkowski S, Giorgis F, Goodacre R, Graham D, Hardy M, Heck C, Heeg S, Hewitt K, Jamieson L, Keeler A, Krolikowska A, Kuttner C, Lidgi-Guigui N, Lightner C, Lombardi J, Mahajan S, Sabanes NM, Masson JF, Mueller NS, Muhamadali H, Murakoshi K, Popp J, Porter M, Reich S, Schatz G, Tian ZQ, Tripathi A, Van Duyne R, Wang XP, Wark A, Willets K, and Willner M.
Faraday Discussions 205, 291 (2017)

PUBLICATIONS

41 **Linking classical and molecular optomechanics descriptions of SERS**
Schmidt MK, Esteban R, Benz F, Baumberg JJ, and Aizpurua J.
Faraday Discussions 205, 31 (2017)

42 **Analytical SERS: general discussion**
Aitchison H, Aizpurua J, Arnolds H, Baumberg J, Bell S, Bonifacio A, Chikkaraddy R, Dawson P, de Nijs B, Deckert V, Delfino I, Di Martino G, Eremina O, Faulds K, Fountain A, Gawinkowski S, Castano MG, Goodacre R, Gracie J, Graham D, Guicheteau J, Hardwick L, Hardy M, Heck C, Jamieson L, Kamp M, Keeler A, Kuttner C, Langer J, Mahajan S, Sabanes NM, Murakoshi K, Porter M, Schatz G, Schlucker S, Tian ZQ, Tripathi A, Van Duyne R, and Vikesland P.
Faraday Discussions 205, 561 (2017)

43 **Electronic Structure and Magnetic Anisotropy in Lanthanoid Singleton Magnets with C-3 Symmetry: The Ln (trenovan) Series**
Lucaccini E, Baldovi JJ, Chelazzi L, Barra A, Grepioni F, Costes JP, and Sorace L
Inorganic Chemistry 56, 4728 (2017)

44 **Ab-initio Modeling of Plasmons in Metal-semiconductor Bilayer Transition-metal Dichalcogenide Heterostructures**
Sen HS, Xian LD, da Jornada FH, Louie SG, and Rubio A.
Israel journal of Chemistry 57, 540 (2017)

45 **Magnetic extension as an efficient method for realizing the quantum anomalous hall state in topological insulators**
Otrokov MM, Menshchikova TV, Rusinov IP, Vergniory MG, Kuznetsov VM, and Chulkov EV.
JETP Letters 105, 297 (2017)

46 **Effect of Deformation on the Electronic Structure and Topological Properties of the A(II)Mg(2)Bi(2) (A(II) = Mg,Ca,Sr,Ba) Compounds**
Petrov EK, Silkin IV, Koroteev YM, and Chulkov EV.
JETP Letters 105, 502 (2017)

47 **Electronic States with Nontrivial Topology in Dirac Materials**
Turkevich RV, Perov AA, Protogenov AP, and Chulkov EV.
JETP Letters 106, 188 (2017)

48 **Competing rhombohedral and monoclinic crystal structures in MnPn(2)Ch(4) compounds: An ab-initio study**
Eremeev SV, Otrokov MM, and Chulkov EV.
Journal of Alloys and Compounds 709, 172 (2017)

49 **Electron refraction at lateral atomic interfaces**
Abd El-Fattah ZM, Kher-Elden MA, Yassin O, El-Okr MM, Ortega JE, and García de Abajo FJ.
Journal of Applied Physics 122, 195306 (2017)

50 **From tunneling to contact in a magnetic atom: The non-equilibrium Kondo effect**
Choi DJ, Abufager P, Limot L, and Lorente N.
Journal of Chemical Physics 146, 092309 (2017)

PUBLICATIONS

51 **A tunable electronic beam splitter realized with crossed graphene nanoribbons**
Brandimarte P, Engelund M, Papior N, Garcia-Lekue A, Frederiksen T, and Sanchez-Portal D.
Journal of Chemical Physics 146, 092318 (2017)

52 **On the non-exponentiality of the dielectric Debye-like relaxation of monoalcohols**
Arrese-Igor S, Alegria A, and Colmenero J.
Journal of Chemical Physics 146, 114502 (2017)

53 **Complex nonequilibrium dynamics of stacked polystyrene films deep in the glassy state**
Boucher VM, Cangialosi D, Alegria A, and Colmenero J.
Journal of Chemical Physics 146, 20 (2017)

54 **Communication: Hot-atom abstraction dynamics of hydrogen from tungsten surfaces: The role of surface structure**
Galparsoro O, Busnengo HF, Juaristi JI, Crespos C, Alducin M, and Larregaray P.
Journal of Chemical Physics 147, 121103 (2017)

55 **Versatile H2O2-driven mixed aerogel synthesis from CdTe and bimetallic noble metal nanoparticles**
Wendt R, Marker B, Dubavik A, Herrmann AK, Wollgarten M, Rakovich YP, Eychmuller A, Rademann K, and Hendel T.
Journal of Materials Chemistry C 5, 10251 (2017)

56 **Designing 3D topological insulators by 2D-Xene (X = Ge, Sn) sheet functionalization in GaGeTe-type structures**
Pielnhofer F, Menshchikova TV, Rusinov IP, Zeugner A, Sklyadneva IY, Heid R, Bohnen KP, Golub P, Baranov AI, Chulkov EV, Pfitzner A, Ruck M, and Isaeva A.
Journal of Materials Chemistry C 5, 4752 (2017)

57 **Synthesis of transparent Er-doped fluorotellurite glass-ceramics through controlled crystallization**
Morea R, Teddy Fernandez T, Fernandez J, Balda R, and Gonzalo J.
Journal of Materials Science 28, 7000 (2017)

58 **Transient and Stable Profiles During Anisotropic Wet Etching of Quartz**
Xing Y, Gosalvez MA, Zhang H, Li Y, and Qiu XL.
Journal of Microelectromechanical Systems 26, 1063 (2017)

59 **Synthesis and properties of Nd-doped oxynitride phosphate laser glasses**
Muñoz F, Saitoh A, Jiménez-Riobóo RJ, and Balda R.
Journal of Non-Crystalline Solids 473, 125 (2017)

60 **Transformation of Amorphous Carbon Clusters to Fullerenes**
Sinitsa AS, Lebedeva IV, Popov AM, and Knizhnik AA.
Journal of Physical Chemistry C 121, 13396 (2017)

61 **Vibrational Excitation of H-2 Scattering from Cu(111): Effects of Surface Temperature and of Allowing Energy Exchange with the Surface**
Kroes GJ, Juaristi JI, and Alducin M.
Journal of Physical Chemistry C 121, 13617 (2017)

PUBLICATIONS

62 **On-Surface Synthesis of a Pure and Long-Range-Ordered Titanium(IV)-Porphyrin Contact Layer on Titanium Dioxide**
Lovat G, Forrer D, Abadia M, Dominguez M, Casarin M, Rogero C, Vittadini A, and Floreano L.
Journal of Physical Chemistry C 121, 13738 (2017)

63 **Structural and Vibrational Properties of the TiOPc Monolayer on Ag(111)**
Fernandez L, Thussing S, Manz A, Witte G, Brion-Rios AX, Cabrera-Sanfelix P, Sanchez-Portal D, and Jakob P.
Journal of Physical Chemistry C 121, 1608 (2017)

64 **Interaction of Cobalt Atoms, Dimers, and Coo Clusters with Circumcoronene: A Theoretical Study**
Alonso-Lanza T, Mananes A, and Ayuela A.
Journal of Physical Chemistry C 121, 18900 (2017)

65 **Stereodynamics of Diatom Formation through Eley-Rideal Abstraction**
Galparsoro O, Juaristi JI, Crespos C, Alducin M, and Larregaray P.
Journal of Physical Chemistry C 121, 19849 (2017)

66 **Microscopic Origin of the Apparent Activation Energy in Diffusion-Mediated Monolayer Growth of Two-Dimensional Materials**
Gosalvez MA, and Alberdi-Rodriguez J.
Journal of Physical Chemistry C 121, 20315 (2017)

67 **Manipulating the Magnetic Moment of Palladium Clusters by Adsorption and Dissociation of Molecular Hydrogen**
Lopez MJ, Blanco-Rey M, Juaristi JI, Alducin M, and Alonso JA.
Journal of Physical Chemistry C 121, 20756 (2017)

68 **Pressure-Induced Stable Li5P for High-Performance Lithium-Ion Batteries**
Zhao ZY, Liu LL, Yu T, Yang GC, and Bergara A.
Journal of Physical Chemistry C 121, 21199 (2017)

69 **Submonolayer Adsorption of Potassium on Reconstructed and Unreconstructed Cu(110): Structure and Phonons**
Borisova SD, Rusina GG, Eremeev SV, and Chulkov EV.
Journal of Physical Chemistry C 121, 22969 (2017)

70 **Transport Properties of Co in Cu(100) from Density Functional Theory Calculations**
Garcia-Fernandez C, Abufager P, and Lorente N.
Journal of Physical Chemistry C 121, 23736 (2017)

71 **Adatom Coadsorption with Three-Dimensional Cyclophanes on Ag(111)**
Scheil K, Lorente N, Bocquet ML, Hess PC, Mayor M, and Berndt R.
Journal of Physical Chemistry C 121, 25303 (2017)

72 **Electronic Structure of Titanylphthalocyanine Layers on Ag(111)**
Lerch A, Fernandez L, Ilyn M, Gastaldo M, Paradinas M, Valbuena MA, Mugarza A, Ibrahim ABM, Sundermeyer J, Hofer U, and Schiller F.
Journal of Physical Chemistry C 121, 25353 (2017)

PUBLICATIONS

73 **Ultrashort Mn-Mn Bonds in Organometallic Complexes**
Alonso-Lanza T, Gonzalez JW, Aguilera-Granja F, and Ayuela A.
Journal of Physical Chemistry C 121, 25554 (2017)

74 **Exploring the Relation Between Intramolecular Conjugation and Band Dispersion in One-Dimensional Polymers**
Garcia-Fernandez C, Sierda E, Abadia M, Bugenhagen B, Prosenc MH, Wiesendanger R, Bazarnik M, Ortega JE, Brede J, Matito E, and Arnau A.
Journal of Physical Chemistry C 121, 27118 (2017)

75 **Laterally Selective Oxidation of Large-Scale Graphene with Atomic Oxygen**
Kapitanova OO, Kataev EY, Usachov DY, Sirotina AP, Belova AI, Sezen H, Amati M, Al-Hada M, Gregoratti L, Barinov A, Cho HD, Kang TW, Panin GN, Vyalikh D, Itkis DM, and Yashina LV.
Journal of Physical Chemistry C 121, 27915 (2017)

76 **Symmetry, Shape, and Energy Variations in Frontier Molecular Orbitals at Organic/Metal Interfaces: The Case of F(4)TCNQ**
Borghetti P, Sarasola A, Merino-Diez N, Vasseur G, Floreano L, Lobo-Checa J, Arnau A, de Oteyza DG, and Ortega JE.
Journal of Physical Chemistry C 121, 28412 (2017)

77 **Step-doubling at Vicinal Ni(111) Surfaces Investigated with a Curved Crystal**
Ityn M, Magana A, Walter AL, Lobo-Checa J, de Oteyza DG, Schiller F, and Ortega JE.
Journal of Physical Chemistry C 121, 3880 (2017)

78 **Theoretical Insights into Unexpected Molecular Core Level Shifts: Chemical and Surface Effects**
Sarasola A, Abadia M, Rogero C, and Garcia-Lekue A
Journal of Physical Chemistry Letters 8, 5718 (2017)

79 **Ground- and excited-state scattering potentials for the stopping of protons in an electron gas**
Matias F, Fadanelli RC, Grande PL, Koval NE, Muino RD, Borisov AG, Arista NR, and Schiwietz G.
Journal of Physics B-atomic Molecular and Optical Physics 50, 185201 (2017)

80 **Odd-frequency superconductivity induced in topological insulators with and without hexagonal warping**
Vasenko AS, Golubov AA, Silkin VM, and Chulkov EV.
Journal of Physics- Condensed Matter 29, 295502 (2017)

81 **Selective excitation in transparent oxyfluoride glass-ceramics doped with Nd3+**
Gorni G, Velázquez JJ, Mather GC, Durán A, Chen G, Sundararajan M, Balda R, Fernández J, and Pascual MJ.
Journal of the European Ceramic Society 37, 1695 (2017)

82 **Whispering gallery mode hybridization in photonic molecules**
Li YC, Abolmaali F, Allen KW, Limberopoulos NI, Urbas A, Rakovich Y, Maslov AV, and Astratov VN.
Laser & Photonics Reviews 11, 1600278 (2017)

83 **Speckle-free near-infrared imaging using a Nd3+ random laser source**
Barredo-Zuriarrain M, Iparraguirre I, Fernández J, Azkargorta J, and Balda R
Laser Phys. Lett. 14, 106201 (2017)

PUBLICATIONS

84 **The Complex Amorphous Phase in Poly(butylene succinate-ran-butylene azelate) Isodimorphic Copolyesters**
Arandia I, Mugica A, Zubitur M, Mincheva R, Dubois P, Muller AJ, and Alegria A.
Macromolecules 50, 1569 (2017)

85 **The Role of the Topological Constraints in the Chain Dynamics in All Polymer Nanocomposites**
Bacova P, Lo Verso F, Arbe A, Colmenero J, Pomposo JA, and Moreno AJ.
Macromolecules 50, 1719 (2017)

86 **Folding Single Chains to Single-Chain Nanoparticles via Reversible Interactions: What Size Reduction Can One Expect?**
Pomposo JA, Rubio-Cervilla J, Moreno AJ, Lo Verso F, Bacova P, Arbe A, and Colmenero J.
Macromolecules 50, 1732 (2017)

87 **Detection, Quantification, and "Click-Scavenging" of Impurities in Cyclic Poly(glycidyl phenyl ether) Obtained by Zwitterionic Ring-Expansion Polymerization with B(C6F5)(3)**
Haque FM, Alegria A, Grayson SM, and Barroso-Bujans F.
Macromolecules 50, 1870 (2017)

88 **Size of Elastic Single-Chain Nanoparticles in Solution and on Surfaces**
De-La-Cuesta J, Gonzalez E, Moreno AJ, Arbe A, Colmenero J, and Pomposo JA.
Macromolecules 50, 6323 (2017)

89 **Supramolecular Self-Assembly of Monocarboxydecyl-Terminated Dimethylsiloxane Oligomer**
Martinez-Rugerio G, Arbe A, Colmenero J, and Alegria A.
Macromolecules 50, 8688 (2017)

90 **Formation of Surface and Quantum-Well States in Ultra Thin Pt Films on the Au(111) Surface**
Silkin IV, Koroteev YM, Echenique PM, and Chulkov EV.
Materials 10, 1409 (2017)

91 **Spectral Selectivity of Plasmonic Interactions between Individual Up-Converting Nanocrystals and Spherical Gold Nanoparticles**
Piatkowski D, Schmidt MK, Twardowska M, Nyk M, Aizpurua J, and Mackowski S.
Materials 10, 905 (2017)

92 **Advances in Fluorescent Single-Chain Nanoparticles**
De-La-Cuesta J, Gonzalez E, and Pomposo JA.
Molecules 22, 1819 (2017)

93 **Spin Orientation of Two-Dimensional Electrons Driven by Temperature-Tunable Competition of Spin-Orbit and Exchange-Magnetic Interactions**
Generalov A, Otrokov MM, Chikina A, Kliemt K, Kummer K, Hoppner M, Guttler M, Seiro S, Fedorov A, Schulz S, Danzenbacher S, Chulkov EV, Geibel C, Laubschat C, Dudin P, Hoesch M, Kim T, Radovic M, Shi M, Plumb NC, Krellner C, and Vyalikh DV.
Nano Letters 17,12,712 811 (2017)

PUBLICATIONS

94 **Formation of Nickel Clusters Wrapped in Carbon Cages: Toward New Endohedral Metallofullerene Synthesis**
Sinitsa AS, Chamberlain TW, Zoberbier T, Lebedeva IV, Popov AM, Knizhnik AA, McSweeney RL, Biskupek J, Kaiser U, and Khlobystov AN.
Nano Letters 17, 1082 (2017)

95 **Strong Magneto-Optical Response of Nonmagnetic Organic Materials Coupled to Plasmonic Nanostructures**
Melnikau D, Govyadinov AA, Sanchez-Iglesias A, Grzelczak M, Liz-Marzan LM, and Rakovich YP.
Nano Letters 17, 1808 (2017)

96 **Efficient Spin-Flip Excitation of a Nickelocene Molecule**
Ormaza M, Bachellier N, Faraggi MN, Verlhac B, Abufager P, Ohresser P, Joly L, Romeo M, Scheurer F, Bocquet ML, Lorente N, and Limot L.
Nano Letters 17, 1877 (2017)

97 **Large-Gap Magnetic Topological Heterostructure Formed by Subsurface Incorporation of a Ferromagnetic Layer**
Hirahara T, Eremeev SV, Shirasawa T, Okuyama Y, Kubo T, Nakanishi R, Akiyama R, Takayama A, Hajiri T, Ideta S, Matsunami M, Sumida K, Miyamoto K, Takagi Y, Tanaka K, Okuda T, Yokoyama T, Kimura S, Hasegawa S, and Chulkov EV.
Nano Letters 17, 3493 (2017)

98 **Quantum Dots Embedded in Graphene Nanoribbons by Chemical Substitution**
Carbonell-Sanroma E, Brandimarte P, Balog R, Corso M, Kawai S, Garcia-Lekue A, Saito S, Yamaguchi S, Meyer E, Sanchez-Portal D, and Pascual JI.
Nano Letters 17, 50 (2017)

99 **Building Complex Kondo Impurities by Manipulating Entangled Spin Chains**
Choi DJ, Robles R, Yan SC, Burgess JAJ, Rolf-Pissarczyk S, Gauyacq JP, Lorente N, Ternes M, and Loth S.
Nano Letters 17, 6203 (2017)

100 **Design of active and stable oxygen reduction reaction catalysts by embedding Co (x) O (y) nanoparticles into nitrogen-doped carbon**
Yang F, Abadia M, Chen CQ, Wang WK, Li L, Zhang LB, Rogero C, Chuvilin A, and Knez M.
Nano Research 10, 97 (2017)

101 **Advances in Single-Chain Nanoparticles for Catalysis Applications**
Rubio-Cervilla J, Gonzalez E, and Pomposo JA.
Nanomaterials 7, 341 (2017)

102 **Very high temperature tiling of tetraphenylporphyrin on rutile TiO2(110)**
Lovat G, Forrer D, Abadia M, Dominguez M, Casarin M, Rogero C, Vittadini A, and Floreano L.
Nanoscale 9, 11694 (2017)

103 **Structural stability and uniformity of magnetic Pt-13 nanoparticles in NaY zeolite**
Di Paola C, Pavan L, D'Agosta R, and Baletto F.
Nanoscale 9, 15658 (2017)

PUBLICATIONS

104 **Self-texturizing electronic properties of a 2-dimensional GdAu2 layer on Au(111): the role of out-of-plane atomic displacement**
Correa A, Camellone MF, Barragan A, Kumar A, Cepek C, Pedio M, Fabris S, and Vitali L.
Nanoscale 9, 17342 (2017)

105 **A classical description of subnanometer resolution by atomic features in metallic structures**
Trautmann S, Aizpurua J, Gotz I, Undisz A, Dellith J, Schneidewind H, Rettenmayr M, and Deckert V.
Nanoscale 9, 391 (2017)

106 **Immobilization of pH-sensitive CdTe Quantum Dots in a Poly(acrylate) Hydrogel for Microfluidic Applications**
Franke M, Leubner S, Dubavik A, George A, Savchenko T, Pini C, Frank P, Melnikau D, Rakovich Y, Gaponik N, Eychmuller A, and Richter A.
Nanoscale Research Letters 12, 314 (2017)

107 **Creating stable Floquet-Weyl semimetals by laser-driving of 3D Dirac materials**
Hubener H, Sentef MA, De Giovannini U, Kemper AF, and Rubio A.
Nature Communications 8, 13940 (2017)

108 **Plasmonic photoluminescence for recovering native chemical information from surface-enhanced Raman scattering**
Lin KQ, Yi, Zhong JH, Hu S, Liu BJ, Liu JY, Zong C, Lei ZC, Wang X, Aizpurua J, Esteban R, and Ren B.
Nature Communications 8, 14891 (2017)

109 **Magnetically-driven colossal supercurrent enhancement in InAs nanowire Josephson junctions**
Tiira J, Strambini E, Amado M, Roddaro S, San-Jose P, Aguado R, Bergeret FS, Ercolani D, Sorba L, and Giazotto F.
Nature Communications 8, 14984 (2017)

110 **Mapping the orbital structure of impurity bound states in a superconductor**
Choi DJ, Rubio-Verdú C, de Bruijckere J, M. Ugeda M, Lorente N, and Pascual JI.
Nature Communications 8, 15175 (2017)

111 **Sub-nanometre control of the coherent interaction between a single molecule and a plasmonic nanocavity**
Zhang Y, Meng QS, Zhang L, Luo Y, Yu YJ, Yang B, Zhang Y, Esteban R, Aizpurua J, Luo Y, Yang JL, Dong ZC, and Hou JG.
Nature Communications 8, 15225 (2017)

112 **Controlled spin switching in a metallocene molecular junction**
Ormaza M, Abufager P, Verlhac B, Bachellier N, Bocquet ML, Lorente N, and Limot L.
Nature Communications 8, 1974 (2017)

113 **Precise engineering of quantum dot array coupling through their barrier widths**
Piquero-Zulaica I, Lobo-Checa J, Sadeghi A, Abd El-Fattah ZM, Mitsui C, Okamoto T, Pawlak R, Meier T, Arnau A, Ortega JE, Takeya J, Goedecker S, Meyer E, and Kawai S.
Nature Communications 8, 787 (2017)

PUBLICATIONS

114 **Probing low-energy hyperbolic polaritons in van der Waals crystals with an electron microscope**
Govyadinov AA, Konecna A, Chuvilin A, Velez S, Dolado I, Nikitin AY, Lopatin S, Casanova F, Hueso LE, Aizpurua J, and Hillenbrand R.
Nature Communications 8, 95 (2017)

115 **Phase coexistence and electric-field control of toroidal order in oxide superlattices**
Damodaran AR, Clarkson JD, Hong Z, Liu H, Yadav AK, Nelson CT, Hsu SL, McCarter MR, Park KD, Kravtsov V, Farhan A, Dong Y, Cai Z, Zhou H, Aguado-Puente P, Garcia-Fernandez P, Iniguez J, Junquera J, Scholl A, Raschke MB, Chen LQ, Fong DD, Ramesh R, and Martin LW.
Nature Materials 16, 1003 (2017)

116 **Charge-transfer states and optical transitions at the pentacene-TiO2 interface**
Ljungberg MP, Vanska O, Koval P, Koch SW, Kira M, and Sanchez-Portal D.
New Journal of Physics 19, 033019 (2017)

117 **Influence of grain size and Nd3+ concentration on the stimulated emission of LiLa1-xNdxP4O12 crystal powders**
Azkargorta J, Marciniak L, Iparraguirre I, Balda R, Strek W, Barredo-Zuriarrain M, García-Revilla S, and Fernandez J.
Optical Materials 63, 46-50 (2017)

118 **Determination of reverse cross-relaxation process constant in Tm-doped glass by H-3(4) fluorescence decay tail fitting**
Albalawi A, Varas S, Chiasera A, Gevabi H, Albalawi W, Blanc W, Balda R, Lukowiak A, Ferrari M, and Taccheo S.
Optical Materials Express 7, 3760 (2017)

119 **Self-assembled flat-faceted nanoparticles chains as a highly-tunable platform for plasmon-enhanced spectroscopy in the infrared**
Aguirregabiria G, Aizpurua J, and Esteban R.
Optics Express 25, 13760 (2017)

120 **Edge stacking dislocations in two-dimensional bilayers with a small lattice mismatch**
Lebedeva IV, Knizhnik AA, and Popov AM.
Physica E-Low-Dimensional Systems & Nanostructures 90, 49 (2017)

121 **Complex magnetic orders in small cobalt-benzene molecules**
Gonzalez JW, Alonso-Lanza T, Delgado F, Aguilera-Granja F, and Ayuela A.
Physical Chemistry Chemical Physics 19, 14854 (2017)

122 **Molecular dynamic heterogeneity in relation to free volume and relaxation dynamics in organic glass-formers: oligomeric cis-1,4-poly(isoprene)**
Svajdlenkova H, Arrese-Igor S, Nogellova Z, Alegria A, and Bartos J.
Physical Chemistry Chemical Physics 19, 15215 (2017)

123 **Kinetic differences in the intercalation of linear and cyclic penta(ethylene oxide)s into graphite oxide leading to separation by topology**
Barroso-Bujans F, and Alegria A.
Physical Chemistry Chemical Physics 19, 18366 (2017)

PUBLICATIONS

124 **Dissociative adsorption dynamics of nitrogen on a Fe(111) surface**
Nosir MA, Martin-Gondre L, Bocan GA, and Muino RD.
Physical Chemistry Chemical Physics 19, 24626 (2017)

125 **Investigation of the dynamics of aqueous proline solutions using neutron scattering and molecular dynamics simulations**
de Molina PM, Alvarez F, Frick B, Wildes A, Arbe A, and Colmenero J.
Physical Chemistry Chemical Physics 19, 27739 (2017)

126 **Adsorption dynamics of molecular nitrogen at an Fe(111) surface**
Nosir MA, Martin-Gondre L, Bocan GA, and Muino RD.
Physical Chemistry Chemical Physics 19, 7370 (2017)

127 **Electronic non-adiabatic dynamics in enhanced ionization of isotopologues of hydrogen molecular ions from the exact factorization perspective**
Khosravi E, Abedi A, Rubio A, and Maitra NT.
Physical Chemistry Chemical Physics 19, 8269 (2017)

128 **Reaching the ideal glass transition by aging polymer films**
Boucher VM, Cangialosi D, Alegria A, and Colmenero J.
Physical Chemistry Chemical Physics 19, 961 (2017)

129 **Intrinsic spin Hall conductivity in three-dimensional topological insulator/normal insulator heterostructures**
Men'shov VN, Shvets IA, Tugushev VV, and Chulkov EV.
Physical Review B 96, 075302 (2017)

130 **Vicinage effect in the energy loss of H-2 dimers: Experiment and calculations based on time-dependent density-functional theory**
Koval NE, Borisov AG, Rosa LFS, Stori EM, Dias JF, Grande PL, Sanchez-Portal D, and Muino RD.
Physical Review A 95, 062707 (2017)

131 **Metal-insulator transition in disordered systems from the one-body density matrix**
Olsen T, Resta R, and Souza I.
Physical Review B 95, 045109 (2017)

132 **Coherent transport properties of a three-terminal hybrid superconducting interferometer**
Vischi F, Carrega M, Strambini E, D'Ambrosio S, Bergeret FS, Nazarov YV, and Giazotto F.
Physical Review B 95, 054504 (2017)

133 **Surface theorem for the Chern-Simons axion coupling**
Olsen T, Taherinejad M, Vanderbilt D, and Souza I.
Physical Review B 95, 075137 (2017)

134 **RKKY oscillations in the spin relaxation rates of atomic-scale nanomagnets**
Delgado F, and Fernandez-Rossier J.
Physical Review B 95, 075413 (2017)

PUBLICATIONS

135 **h-AlN-Mg(OH)(2) van derWaals bilayer heterostructure: Tuning the excitonic characteristics**
Bacaksiz, C, Dominguez A, Rubio A, Senger RT, and Sahin H.
Physical Review B 95, 075423 (2017)

136 **Quantum transport simulation scheme including strong correlations and its application to organic radicals adsorbed on gold**
Droghetti A, and Rungger I.
Physical Review B 95, 085131 (2017)

137 **Femtosecond laser induced desorption of H-2, D-2, and HD from Ru(0001): Dynamical promotion and suppression studied with ab initio molecular dynamics with electronic friction**
Juaristi JI, Alducin M, and Saalfrank P.
Physical Review B 95, 125439 (2017)

138 **Valence instability in the bulk and at the surface of the antiferromagnet SmRh2Si2**
Chikina A, Generalov A, Kummer K, Guttler M, Antonov VN, Kucherenko Y, Kliemt K, Krellner C, Danzenbacher S, Kim T, Dudin P, Geibel C, Laubschat C, and Vyalikh DV.
Physical Review B 95, 155127 (2017)

139 **Instability of the topological surface state in Bi2Se3 upon deposition of gold**
Polyakov A, Tusche C, Ellguth M, Crozier ED, Mohseni K, Otrokov MM, Zubizarreta X, Vergniory MG, Geilhufe M, Chulkov EV, Ernst A, Meyerheim HL, and Parkin SSP.
Physical Review B 95, 180202 (2017)

140 **Insight into the temperature dependent properties of the ferromagnetic Kondo lattice YbNiSn**
Generalov A, Sokolov DA, Chikina A, Kucherenko Y, Antonov VN, Bekenov LV, Patil S, Huxley AD, Allen JW, Matho K, Kummer K, Vyalikh DV, and Laubschat C.
Physical Review B 95, 184433 (2017)

141 **Anomalous current in diffusive ferromagnetic Josephson junctions**
Silaev MA, Tokatly IV, and Bergeret FS.
Physical Review B 95, 184508 (2017)

142 **Geometric and electronic structure of the Cs-doped Bi2Se3(0001) surface**
Otrokov MM, Ernst A, Mohseni K, Fulara H, Roy S, Castro GR, Rubio-Zuazo J, Ryabishchenkova AG, Kokh KA, Tereshchenko OE, Aliev ZS, Babanly MB, Chulkov EV, Meyerheim HL, and Parkin SSP.
Physical Review B 95, 205429 (2017)

143 **Nontrivial topology of cubic alkali bismuthides**
Rusinov IP, Sklyadneva IY, Heid R, Bohnen KP, Petrov EK, Koroteev YM, Echenique PM, and Chulkov EV.
Physical Review B 95, 224305 (2017)

144 **Quantum-size effects in the loss function of Pb(111) thin films: An ab initio study**
Zubizarreta X, Chulkov EV, Chernov IP, Vasenko AS, Aldazabal I, and Silkin VM.
Physical Review B 95, 235405 (2017)

145 **Quantum description of the optical response of charged monolayer-thick metallic patch nanoantennas**
Herrera MZ, Kazansky AK, Aizpurua J, and Borisov AG.
Physical Review B 95, 245413 (2017)

PUBLICATIONS

146 **Proximity Eliashberg theory of electrostatic field-effect doping in superconducting films**
Ummarino GA, Piatti E, Daghero D, Gonnelli RS, Sklyadneva IY, Chulkov EV, and Heid R.
Physical Review B 96, 064509 (2017)

147 **Composite Weyl nodes stabilized by screw symmetry with and without time-reversal invariance**
Tsirkin SS, Souza I, and Vanderbilt D.
Physical Review B 96, 045102 (2017)

148 **Ab initio study of the electron energy loss function in a graphene-sapphire-graphene composite system**
Despoja V, Djordjevic T, Karbunar L, Radovic I, and Miskovic ZL.
Physical Review B 96, 075433 (2017)

149 **Stacking in incommensurate graphene/hexagonal-boron-nitride heterostructures based on ab initio study of interlayer interaction**
Lebedev AV, Lebedeva IV, Popov AM, and Knizhnik AA.
Physical Review B 96, 085432 (2017)

150 **Energy loss and surface temperature effects in ab initio molecular dynamics simulations: N adsorption on Ag(111) as a case study**
Novko D, Loncaric I, Blanco-Rey M, Juaristi JI, and Alducin M.
Physical Review B 96, 085437 (2017)

151 **Modeling of laser-pulse induced water decomposition on two-dimensional materials by simulations based on time-dependent density functional theory**
Miyamoto Y, Zhang H, Cheng XL, and Rubio A.
Physical Review B 96, 115451 (2017)

152 **Two- and three-dimensional topological phases in BiTeX compounds**
Eremeev SV, Nechaev IA, and Chulkov EV.
Physical Review B 96, 155309 (2017)

153 **Regularities of the quantum spin Hall phase formation in three-dimensional tetradymite-like topological insulator thin films**
Menshchikova TV, Silkina OY, Silkin IV, Kuznetsov VM, and Chulkov EV.
Physical Review B 96, 165441 (2017)

154 **Spectroscopic perspective on the interplay between electronic and magnetic properties of magnetically doped topological insulators**
Krieger JA, Chang CZ, Husanu MA, Sostina D, Ernst A, Otrokov MM, Prokscha T, Schmitt T, Suter A, Vergniory MG, Chulkov EV, Moodera JS, Strocov VN, and Salman Z.
Physical Review B 96, 18 (2017)

155 **Anharmonicity and the isotope effect in superconducting lithium at high pressures: A first-principles approach**
Borinaga M, Aseginolaza U, Errea I, Calandra M, Mauri F, and Bergara A.
Physical Review B 96, 184505 (2017)

PUBLICATIONS

156 **Impact of stoichiometry and disorder on the electronic structure of the PbBi2Te4-xSex topological insulator**
Shvets IA, Klimovskikh II, Aliev ZS, Babanly MB, Sanchez-Barriga J, Krivenkov M, Shikin AM, and Chulkov EV.
Physical Review B 96, 235124 (2017)

157 **Electrical control of the light absorption in quantum-well functionalized junctions between thin metallic films**
Marinica DC, Kazansky AK, and Borisov AG.
Physical Review B 96, 245407 (2017)

158 **Electronic Stopping of Slow Protons in Transition and Rare Earth Metals: Breakdown of the Free Electron Gas Concept**
Roth D, Bruckner B, Moro MV, Gruber S, Goebl D, Juaristi JI, Alducin M, Steinberger R, Duchoslav J, Primetzhofer D, and Bauer P.
Physical Review Letters 118, 103401 (2017)

159 **Transport Properties of an Electron-Hole Bilayer in Contact with a Superconductor Hybrid Junction**
Bercioux D, Klapwijk TM, and Bergeret FS.
Physical Review Letters 119, 067001 (2017)

160 **Strong Anisotropic Interaction Controls Unusual Sticking and Scattering of CO at Ru(0001)**
Loncaric I, Fuchsel G, Juaristi JI, and Saalfrank P.
Physical Review Letters 119, 146101 (2017)

161 **Electronic stopping of slow protons in oxides: scaling properties**
Roth, D, Bruckner B, Undeutsch G, Paneta V, Mardare AI, McGahan CL, Dosmailov M, Juaristi JI, Alducin M, Pedarnig JD, Haglund RF, Primetzhofer D, and Bauer P.
Physical Review Letters 119, 163401 (2017)

162 **Stable carbon monosulfide nanostructures: Chain arrays and monolayers**
Alonso-Lanza T, Aguilera-Granja F, Gonzalez JW, and Ayuela A.
Physical Review Materials 1, 024001 (2017)

163 **Revealing the magnetic proximity effect in EuS/Al bilayers through superconducting tunneling spectroscopy**
Strambini E, Golovach VN, De Simoni G, Moodera JS, Bergeret FS, and Giazotto F.
Physical Review Materials 1, 054402 (2017)

164 **Synthesis, Characterisation and electrospinning of poly(vinyl caprolactam-co-hydroxymethyl acrylamide) to create stimuli-responsive nanofibers**
Gonzalez E, and Frey MW.
Polymer 108, 154 (2017)

165 **Acrylic-based composite latexes containing nano-sized liquid crystalline domains**
Mehravar E, Iturrospe A, Arbe A, Leiza JR, and Asua JM.
Polymer 108, 288 (2017)

PUBLICATIONS

166 **Molecular dynamics of fully biobased poly(butylene 2,5-furanoate) as revealed by broadband dielectric spectroscopy**
Soccio M, Martinez-Tong DE, Alegria A, Munari A, and Lotti N.
Polymer 128, 24 (2017)

167 **Water diffusion and hydrolysis effect on the structure and dynamics of epoxy-anhydride networks**
Capiel G, Miccio LA, Montemartini PE, and Schwartz GA.
Polymer Degradation and Stability 143, 57 (2017)

168 **Non-adiabatic effects in elementary reaction processes at metal surfaces**
Alducin M, Muino RD, and Juaristi JI.
Progress in Surface Science 92, 317 (2017)

169 **Spin decoherence of magnetic atoms on surfaces**
Delgado F, and Fernandez-Rossier J.
Progress in Surface Science 92, 40 (2017)

170 **Phase diagrams in materials science of topological insulators based on metal chalcogenides**
Babanly MB, Chulkov EV, Aliev ZS, Shevelkov AV, and Amiraslanov IR.
Russian Journal of Inorganic Chemistry 62, 1703 (2017)

171 **Angular momentum-induced delays in solid-state photoemission enhanced by intra-atomic interactions**
Siek F, Neb S, Bartz P, Hensen M, Struber C, Fiechter S, Torrent-Sucarrat M, Silkin VM, Krasovskii EE, Kabachnik NM, Fritzsche S, Muino RD, Echenique PM, Kazansky AK, Muller N, Pfeiffer W, and Heinzmann U.
Science 357, 1274 (2017)

172 **Quantum Nuclear Dynamics of Protons within Layered Hydroxides at High Pressure**
Dupuis R, Dolado JS, Benoit M, Surga J, and Ayuela A.
Scientific Reports 7, 4842 (2017)

173 **Electron-phonon coupling in topological surface states: The role of polar optical modes**
Heid R, Sklyadneva IY, and Chulkov EV.
Scientific Reports 7, 1095 (2017)

174 **Giant Magnetic Band Gap in the Rashba-Split Surface State of Vanadium-Doped BiTeI: A Combined Photoemission and Ab Initio Study**
Klimovskikh, II, Shikin AM, Otrokov MM, Ernst A, Rusinov IP, Tereshchenko OE, Golyashov VA, Sanchez-Barriga J, Varykhalov AY, Rader O, Kokh KA, and Chulkov EV.
Scientific Reports 7, 3353 (2017)

175 **Quantum spin Hall insulators in centrosymmetric thin films composed from topologically trivial BiTeI trilayers**
Nechaev IA, Eremeev SV, Krasovskii EE, Echenique PM, and Chulkov EV.
Scientific Reports 7, 43666 (2017)

PUBLICATIONS

176 **Spin-resolved band structure of heterojunction Bi-bilayer/3D topological insulator in the quantum dimension regime in annealed Bi2Te2.4Se0.6**
Klimovskikh II, Sostina D, Petukhov A, Rybkin AG, Eremeev SV, Chulkov EV, Tereshchenko OE, Kokh KA, and Shikin AM.
Scientific Reports 7, 45797 (2017)

177 **Model potential for the description of metal/organic interface states**
Armbrust N, Schiller F, Gudde J, and Hofer U.
Scientific Reports 7, 46561 (2017)

178 **Tuning the Fermi velocity in Dirac materials with an electric field**
Diaz-Fernandez A, Chico L, Gonzalez JW, and Dominguez-Adame F.
Scientific Reports 7, 8058 (2017)

179 **Dynamics of nano-confined water in Portland cement - comparison with synthetic C-S-H gel and other silicate materials**
Goracci G, Monasterio M, Jansson H, and Cerveny S.
Scientific Reports 7, 8258 (2017)

180 **Kinetic Monte Carlo method for the simulation of anisotropic wet etching of quartz**
Zhang H, Xing Y, Li Y, Gosalvez MA, and Qiu XL.
Sensors and Actuators A-Physical 256, 24 (2017)

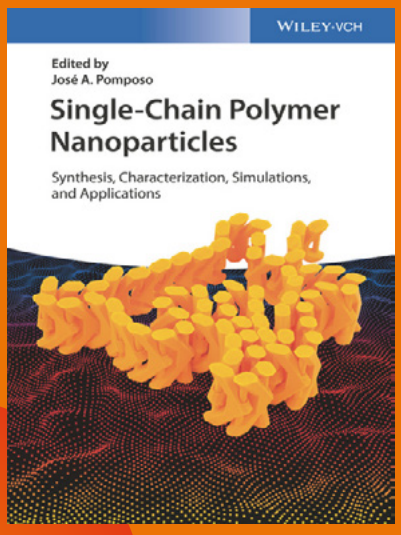
181 **Ionic transport in the amorphous phase of semicrystalline polyethylene oxide thin films**
Martinez-Tong DE, Miccio LA, and Alegria A.
Soft Matter 13, 5597 (2017)

182 **Effects of precursor topology and synthesis under crowding conditions on the structure of single-chain polymer nanoparticles**
Formanek M, and Moreno AJ.
Soft Matter 13, 6430 (2017)

183 **Formation of the bismuth-bilayer film at BiTeCl surface by atomic hydrogen deposition**
Shvets IA, Eremeev SV, and Chulkov EV.
Surface Science 661, 10 (2017)

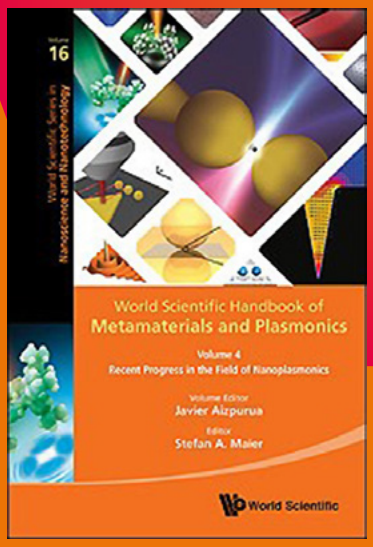
BOOKS

Single-Chain Polymer Nanoparticles



Synthesis, Characterisation, Simulations and Applications

Editor: José A. Pomposo
Wiley-VCH



World Scientific Handbook of Metamaterials and Plasmonics

Volume 4- Recent Progress in the Field of Nanoplasmonics

Volume Editor: Javier Aizpurua
Editor: Stefan A. Maier
World Scientific

TRAINING ACTIVITIES

TRAINING ACTIVITIES

As a joint centre which belongs to the University of the Basque Country (UPV/EHU), the training activity at CFM includes the participation in both the Master and PhD Program through the Department of Material Physics of UPV/EHU, as well as setting complementary training activities, including summer internships for undergraduate students, PhD students seminars and post-doctoral researchers training. All these activities are strongly related and coordinated with the research activity at the different research groups at CFM. We note in the following the main aspects of the training activities at CFM.

MASTER IN NANOSCIENCE

Master in Nanoscience is an official Master program of UPV/EHU (held at CFM headquarters) and co-organised by CFM itself. While attending the Master, the students are also given the opportunity to develop a Master Thesis jointly with one of the groups of the centre on a topic of their choice. Thus, they are exposed for the first time to an environment of excellence in research, where they can learn the methodologies and develop results together with a group devoted to the research on advanced materials.

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 Centres, 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 Thesis successfully defended at CFM in 2017 follows:

- **Electron cooling in nanoscale superconducting structures.**
  Author: Mikel Rouco Martín
- **Tight-binding approach to ballistic transport in multi-terminal 2D nanostructures.**
  Author: Sofia Sanz Wuhl
- **Fluorescent single-chain nanoparticles for sensing and bioimaging applications.**
  Author: Eva Rodriguez Carreira
- **Influence of graphene on tip-enhanced vibrational spectroscopy of a molecular layer.**
  Author: Pavel Gallina
- **Structural Characterisation of Europium layers on Au(111).**
  Author: Jan Dabi Romero
- **Surface studies of Li4Ti5O12 (111) as negative electrode for rechargeable Li-ion batteries.**
  Author: Mikel Iturriza
- **Hybrid materials from J-aggregates and differently-shaped gold nanoparticles: the difference between weak and strong coupling.**
  Author: Nekane Lozano
- **Synthesis, Characterisation and functionalization of Povidone based Single Chain Nanoparticles.**
  Author: Maite del Corte
- **Separation of cyclic and lineal penta(ethylene oxide)s by selective intercalation in Graphite Oxide.**
  Author: Daniel Ruiz Fulgencio

PHD PROGRAM: PHYSICS OF NANOSTRUCTURES AND ADVANCED MATERIALS

"Physics of Nanostructures and Advanced Materials" is a PhD program of UPV/EHU that has been recognised as a highly qualified PhD program by the Spanish Ministry of Education (MEE2011-0591 citation of excellence). Within this program, an average of about 30 to 35 PhD students develop their research fully embedded in the daily life of the research groups in the centre.

The aforementioned PhD program participates in the European Doctorate Program of "Physics and Chemistry of Advanced Materials" (PCAM). PCAM is a European research network of doctoral programs focusing on various aspects of the physics and chemistry of advanced materials.

The list of PhD thesis projects successfully defended at CFM in 2017 follows:

- **Dynamics of diatomic molecules on metal surfaces: O2/Ag(110) and CO/Ru(0001)**
  Author: Ivor Loncaric
  Supervisor: J.I. Juaristi
  25/01/2017

- **Dynamics of biological and non-biological aqueous solutions – Evidence of coupling between the motions of water and solutes**
  Author: Izaskun Letizia Combarro Palacios
  Supervisor: S. Cerveny
  21/06/2017

- **Novel synthesis routes of bioinspired nanoparticles and bio-based films**
  Author: Alejandro Latorre Sánchez
  Supervisor: J. A. Pomposo
  30/06/2017

- **Theoretical Characterisation in the functionalization and design of low dimensional systems: carbon transition metal nanostructures and phosphorene isoelectronic compounds**
  Author: Tomás Alonso Lanza
  Supervisor: A. Ayuela
  30/06/2017

- **Ullmann coupling reaction in unconventional surfaces**
  Author: Mikel Abadia Gutierrez
  Supervisor: C. Rogero and J. Brede
  14/07/2017

- **Morphology and Dynamics of Ice Cristals and the Effect of Proteins**
  Author: Maria Cascajo Castresana
  Supervisor: S. Cerveny and A.M. Bittner
  17/07/2017

- **Ab-Initio Theoretical Study of Electronic Excitations and Optical Properties in Nanostructures**
  Author: Federico Marchesin
  Supervisor: D. Sánchez-Portal
  21/07/2017

- **Propiedades Estructurales y Electrónicas de las Aleaciones Bidimensionales de GdAg2/Ag(111) y de GdAu2/Au(111)**
  Author: Alexander Correa
  Supervisor: L. Vitaly
  07/09/2017

- **Ald processes development for hybrid nanodevices-like nanostructures**
  Author: Mabel Moreno
  Supervisor: J.M. Pitarke
  12/09/2017

- **Quantum Electrodynamical Time-Dependent Density Functional Theory**
  Author: Camila Pellegrini
  Supervisor: A. Rubio and I. Tokatly
  21/09/2017

- **Single-Chain Nanoparticles: Exploring Novel Synthesis Routes, Basic Properties and Potential Applications**
  Author: Marina González
  Supervisor: A. Arbe and J.A. Pomposo
  14/12/2017

PHD INTERNSHIPS ABROAD

A very important aspect of the PhD training program consists of supporting short stays in foreign universities and centres for CFM students. An average of about 6 PhD students per year spend about 2-3 months in some of the best international centres on their topics. This training activity combines aspects of internationalisation and excellence, and has been strongly supported within the last years by CFM. In the following PhD researchers benefit from an internship abroad supported by CFM:

- **Lucía Ortega Álvarez**
  GoodYear Innovation Centre (GIC*L) Colmar Berg (Luxemburg)
  01 March/30 April

- **Jon Rubio Cervilla**
  University of Brisbane (Australia)
  27 September/ 27 December

- **Mattin Urbieta Galarraga**
  University of Houston (USA)
  01 October/ 23 December

- **Tomas Neuman**
  University of Strasbourg (France)
  01 October/ 30 November

- **Unai Aseguinolaza Aguirreche**
  Institut de Nanoscience de Paris (France)
  02 October/ 20 December

POST-DOCTORAL TRAINING

Post-doctoral researchers make extremely valuable contributions to the research activity at CFM, but they are at an early stage of their scientific careers. This means that they still need to acquire further research skills to successfully develop their scientific careers at a later stage. CFM encourages the research groups to hire post-doctoral researchers through internal calls, which support around 2-3 post-doc positions every year. Each research group makes an individual follow-up and training of these young researchers.

UNDERGRADUATE EDUCATION PROGRAM

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.

Summer Internships

Undergraduate students are also offered the possibility to be trained in-situ at CFM, with the opportunity to interact with top quality research groups in summer internships. CFM provided three summer internships to undergraduate students during 2017:

- **Alberto Hijano Mendizabal**
  Group: Nanophysics lab
  Supervisor: Enrique Ortega

- **Iker Castrillo Maestro**
  Group: Polymers and Soft Matter
  Supervisor: Ángel Alegría

- **Usue Aspiazu Iturbe**
  Group: Polymers and Soft Matter
  Supervisor: Josetxo Pomposo

Students Training

During 2017 the following undergraduate students joined a research group at CFM to fulfil their *End of Course Project* or to do a short training stay.

- **Ane Puente Irizar**
  Project title: Síntesis de nanopartículas poliméricas unimoleculares y micelas fluorescents.
  Group: Polymers and Soft Matter
  Supervisor: Josetxo Pomposo and Edurne Gonzalez

- **Anna Oelsch** (short visiting)
  Group: Nanophysics Lab
  Supervisor: Frederik Michael Schiller

- **Ander Arregui Biera** (ongoing project)
  Group: Nanophysics Lab
  Supervisors: Andrés Arnau and Sara Barja

- **Beñat Jimenez Urbieta**
  Project Title: Configuración de un sistema de virtualización en alta disponibilidad basado en Software Libre
  Group: Computing Service
  Supervisor: Iñigo Aldazabal

- **Igor Cortés Cejudo**
  Project Title: Desarrollo de dos módulos de Gwyddion para análisis de defectos lineales en microscopía de efecto túnel
  Group: Computing Service / Nanophysics Lab
  Supervisors: Iñigo Aldazabal and Maxim Ilin

- **Irati Garmendia San Miguel** (ongoing project)
  Group: Nanophysics Lab
  Supervisors: Andrés Arnau and Sara Barja

- **Julen Gorospe Trujillo** (ongoing project)
  Group: Polymers and Soft Matter
  Supervisors: Josetxo Pomposo and Edurne Gonzalez

- **Maitane Romatet Larrañaga** (ongoing project)
  Group: Polymers and Soft Matter
  Supervisor: Josetxo Pomposo and Edurne Gonzalez

Other Training Courses

CFM administration organises health and safety security courses given by CSIC and UPV/EHU central services, as well as IT courses given by the IT responsible (software carpentry) or external experts (COMSOL). Other specialized courses about specific experimental techniques are also organised. Furthermore, a laboratory course on dielectric spectroscopy is successfully organised by CFM researcher Prof. Ángel Alegría, in which 15-20 graduate students and researchers take part yearly.

WORK-SHOPS, CON-FERENCES & SEMINARS

WORKSHOPS, CONFERENCES & SEMINARS

CFM scientists have organised or co-organised several international workshops and conferences during 2017. Many of these meetings have been held in close cooperation with the foundation Donostia Intenational Physics Center (DIPC), which is an example of the excellent results brought by the synergistic collaboration between both institutions.

Moreover, CFM researchers are also regularly invited to give Invited and Plenary talks in international conferences, showing their leadership in their respective fields. During 2017, more than 50 invited talks have been given by CFM researchers. These activities improve dramatically the impact and relevance of the individuals and group research's outcomes.

The list of conferences, workshops and seminars organised or co-organised by CFM researchers during 2017 follows:

INTERNATIONAL CONFERENCES

HPC Knowledge Meeting'17

Co-organised by Jordi Blasco (HPCNow!), Iñigo Aldazabal (CFM, CSIC-UPV/EHU), David Tur (HPCNow!), Txomin Romero (DIPC)
Miramar Royal Palace
(Donostia-San Sebastián, Spain)
15-16/06/2017

13th European Conference on Surface Crystallography and Dynamics (ECSCD – 13)

Co-organised by María Blanco-Rey (chair) (UPV/EHU), Martina Corso (CFM, CSIC/UPV-EHU), Aran García-Lekue (DIPC), Celia Rogero (CFM-CSIC-UPV/EHU, DIPC) and Karmela Alonso Arreche (DIPC)
Miramar Royal Palace
(Donostia-San Sebastián, Spain)
19-21/06/2017

Surfaces and Interfaces

Co-organised by Jose M. Pitarke (CIC nanoGUNE, CFM and UPV/EHU), Shashank Harivyasi (Graz University of Technology, Graz), Mato Knez (CIC nanoGUNE), Morten Madsen (University of Southern Denmark, Sonderborg), Moritz Muller (CFM, CSIC-UPV/EHU), Daniel Sánchez-Portal (CFM, CSIC-UPV/EHU), Weike Wang (CIC nanoGUNE), Julene Lure (CIC nanoGUNE), Itziar Otegui (CIC nanoGUNE) and Katharina Rubahn Rubhan (University of Southern Denmark, Sønderborg)
Miramar Royal Palace
(Donostia-San Sebastián, Spain)
20-23/06/2017

Photo- ElectroCatalysis at the Atomic Scale (PECAS)

Co-organised by Sara Barja (Chair) (Ikerbasque, CFM-UPV/EHU, DIPC), Celia Rogero (CFM-CSIC-UPV/EHU, DIPC), Mato Knez, (Ikerbasque, CiCNanogune) and Karmela Alonso (secretary, DIPC)
Miramar Royal Palace
(Donostia-San Sebastián, Spain)
27-30/06/2017

Frontiers in Quantum Materials and Devices (FQMD)

Co-organised by Vitaly N Golovach (CFM, CSIC-UPV/EHU) and Naomi Brave (CIQM, Harvard University)
Miramar Royal Palace
(Donostia-San Sebastián, Spain)
12-14/07/2017

Quantum Spintronics at Interfaces (Magnon)

Co-organised by Yaroslav Tserkovnyak (University of California, Los Angeles), Vitaly Golovach (DIPC and CFM/EHU) and Sebastián Bergeret (DIPC and CFM/CSIC)
Miramar Royal Palace
(Donostia-San Sebastián, Spain)
4-8/09/2017

Summer School "Frontiers of condensed matter"

Co-organised by Sebastián Bergeret (DIPC, CFM/CSIC), Julia Meyer (Université Grenoble Alpes, France) and Tjerk Oosterkamp (Leiden Institute of Physics/Casimir Research School ,Netherlands)
Les Houches (France)
18-29/09/2017

Exotic New States in Superconducting Devices: The Age of the Interface

Co-organised by Sebastián Bergeret (CFM/CSIC and DIPC), Jason Robinson (University of Cambridge) and Kjetil Hals (JGU Mainz)
Schloß Waldthausen (Mainz, Germany)
25-28/09/2017

Iberian Vacuum Conference, RIVA-X

Co-organised by Javier Barriga (Tekniker, Gipuzkoa), Enrique Ortega (CFM, UPV/EHU), José Ángel Martín-Gago (Institute of Materials Science of Madrid-CSIC), María F. López (Institute of Materials Science of Madrid-CSIC), A. López Vazquez de Parga (University Autonoma of Madrid, Spain), Francisco L. Tabarés (CIEMAT), Carlos Jose Tavares (University of Minho), Miguel Manso (University Autonoma of Madrid, Spain), Miguel Moreno Ugeda (University of the Basque Country, UPV-EHU), Sara Barja Martínez (Ikerbasque, CFM-UPV/EHU, DIPC), María Blanco Rey (DIPC)
Bizkaia Aretoa (Bilbao, Spain)
4-6/10/2017

Modern Trends in Molecular Dynamics and Electron Correlations at Surfaces and Interfaces

Co-organised by Denis Vyalikh (DIPC) Ricardo Díez Muiño (DIPC and CFM, CSIC-UPV/EHU) and Clemens Laubschat (Technische Universität Dresden)
Miramar Royal Palace
(Donostia-San Sebastián, Spain)
27/10/2017

WORKSHOPS

Software Carpentry

Co-organised by Iñigo Aldazabal (CFM, CSIC-UPV/EHU), Mateusz Kuzak (eScience Research Engineer) and Andrés Diaz-Gil (IFT, UAM-CSIC)
Elbira Zipitria Centre-UPV/EHU
(Donostia-San Sebastián, Spain)
28-30/06/2017

CFM Software Carpentry Tracks:

- Python
- Introduction to Version Control with Git
- Introduction to Scientific Python

Organised by Iñigo Aldazabal (CFM, CSIC-UPV/EHU)
CFM (Donostia-San Sebastián, Spain)
2017

PHD STUDENTS SEMINARS AT CFM

Since 2013, a regular series of seminars delivered by PhD students is organised at CFM. This activity continued during 2017. 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. The list of student seminars given in 2017 follows:

- **Probing hyperbolic phonon polaritons in hexagonal boron nitride nanostructures with an electron microscope**
  Andrea Konecna
  13/12/2017

- **Exploring graphene nanoribbons on gold surfaces: Synthesis and electronic structure Characterisation**
  Nestor Merino Diez
  10/05/2017

- **Spin-dependent scattering in a quasi-one-dimensional nanowire**
  Alba Pascual Gil
  10/05/2017

- **Influence of magnetic adatoms on the properties of topological insulators**
  Bernhard Kretz
  26/04/2017

- **Active control of even-harmonic generation using spherical aluminium nanoparticles**
  Garikoitz Aguirregabiria Achutegui
  26/04/2017

- **Precise engineering of quantum dot array coupling through their barrier widths**
  Ignacio Piquero Zulaica
  05/04/2017

- **Computational assessment of the properties of a Cu-based family of photosensitizers**
  Irene Casademont Reig
  05/04/2017

- **Reflectivity from infrared to ultraviolet: an optical approach to metallic hydrogen**
  Miguel Borinaga Treviño
  22/03/2017

- **An array of layers in silicon sulfides: Chainlike and monolayer**
  Tomás Alonso Lanza
  22/03/2017

- **TDDFT and BEM modeling of electron energy loss in metallic nanoparticles**
  Mattin Urbieta Galarraga
  08/03/2017

- **Suppressed electron-phonon interaction due to strong spin-orbit interaction at the Tl/Si(111) surface**
  Peio Garcia
  08/03/2017

- **Nanoplasmonics from large-scale ab initio-calculations: opposite trends in Ag and Na clusters**
  Mark Barbry
  22/02/2017

- **Coupled spin-charge collective oscillations at the Tl/Si(111) surface**
  Jon Lafuente
  22/02/2017

- **Controlling the state of molecular vibrations in resonance surface enhanced Raman scattering**
  Tomas Neuman
  18/01/2017

- **Tunning Confinement effects on thin film of poly(4-tertbutylstyrene) with one free surface**
  Natalia Gutiérrez Pérez de Eulate
  18/01/2017

RESEARCH FUNDING

COMPETITIVE FUNDING FOR RESEARCH PROJECTS

The projects that were in progress during 2017 are listed below according to the source of competitive funding.

BASQUE RESEARCH PROJECTS

- **EJ/GV GRUPO CONSOLIDADO IT578-13**
  Energy Materials: Fundamental developments in AB-initio computational material science
  PI: Rubio Secades, Ángel

- **EJ/GV GRUPO CONSOLIDADO IT621-13**
  Física de nanoestructuras experimental
  PI: Ortega Conejero, Enrique

- **EJ/GV GRUPO CONSOLIDADO IT654-13**
  Polímeros y materia condensada blanda
  PI: Colmenero de León, Juan

- **EJ/GV GRUPO CONSOLIDADO IT756-13**
  Estudio teórico de propiedades estructurales y electrónicas de nanoestructuras y superficies
  PI: Arnau Pino, Andrés

- **EJ/GV, ELKARTEK 2016, KK-2016/00025**
  nG16 FAB - Magneto-elipsómetro para el control de calidad del grafeno
  PI: Souza, Ivo

- **EJ/GV, ELKARTEK 2016, KK-2016/00060**
  SUPER - Advanced manufacturing of nanomaterials by SUPERcritical Fluid Technology
  PI: Cerveny Murcia, Silvina

- **EJ/GV, ELKARTEK 2017, KK-2017/00007**
  NEWHEA - Desarrollo de Aleaciones de Alta Entropía de Baja Densidad
  PI: Alducin Ochoa, Maite

- **EJ/GV, ELKARTEK 2017, KK-2017/00012**
  nG17 - Investigación colaborativa en sistemas de monitorización portable en nanociencia y nanotecnología
  PI: Cerveny Murcia, Silvina

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, RED2017, Exp. 51/17**
  Desarrollo del laboratorio de nanoóptica cuántica
  PI: Molina Terriza, Gabriel

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, RED2017, Exp. 101/17**
  Desarrollo de nanopartículas de Povidona para dosificación de fármacos anticancerosos con detección por fluorescencia
  PI: Pomposo Alonso, Josetxo

- **UPV/EHU, INFRAESTRUCTURA, INF17/08**
  Renovación de un analizador dieléctrico de banda ancha
  PI: Colmenero de León, Juan

SPANISH MINISTRY RESEARCH PROJECTS

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), MAT-2013-46593-C6-4-P**
  Híbridos covalentes en superficies
  PI: Ortega Conejero, Enrique

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), MAT-2013-48246-C2-2-P**
  Efecto del procesamiento sobre la estructura y propiedades de vidrios y vitrocerámicos con aplicaciones fotónicas
  PI: Balda de la Cruz, Rolindes

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), FIS2013-48286-C2-1-P**
  Electronic Processes in Surfaces and Nanostructures
  PI: Ayuela Fernández, Andrés

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), FIS2013-48286-C2-2-P**
  Reactividad, propiedades electrónicas y estructurales de sistemas complejos
  PI: Juaristi Oliden, Joseba Iñaki

- **MEC-MICINN, Contratos Juan de la Cierva-Formación, FPDI-2013-16641**
  Supervisor: Rubio Secades, Ángel

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), FIS2014-55987-P**
  Transporte de espín en estructuras híbridas: metales. Superconductores, semiconductores, grafeno y aislantes topológicos
  PI: Bergeret Sbarbaro, Sebastián

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), MAT2015-63704-P**
  De las nano-partículas blandas unimoleculares a los nano-compuestos totalmente poliméricos
  PI: Colmenero de León, Juan

- **MEC-MICINN, Retos Investigación: Proyectos I+D+i, MAT2015-66888-C3-2-R**
  Magnetismo en la nanoescala: explorando nuevas rutas (Física de dispositivos de spin)
  PI: Lorente Palacios, Nicolás

- **MEC-MICINN, Contratos Ramón y Cajal (RyC), RYC-2015-18281**
  Supervisor: Conejero Ortega, Enrique

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), FIS2016-75862-P**
  Propiedades estructurales, electrónicas y magnéticas de sistemas en escala nanométrica
  PI: Arnau Pino, Andrés

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), FIS2016-76471-P**
  Transferencia de energía en la interacción y dinámica de átomos y moléculas en superficies
  PI: Díez Muiño, Ricardo

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), FIS2016-76617-P**
  Excitaciones electrónicas en superficies y nanoestructuras
  PI: Ayuela Fernández, Andrés

- **MEC-MICINN, Retos Investigación: Proyectos I+D+i, MAT2016-78293-C6-4-R**
  Teoría de nanoestructuras moleculares funcionales para dispositivos optoelectrónicos
  PI: Sánchez Portal, Daniel

- **MEC-MICINN, Retos Investigación: Proyectos I+D+i, MAT2016-78293-C6-5-R**
  Nanoestructuras moleculares funcionales para dispositivos optoelectrónicos: Guiando reacciones en superficies
  PI: Rogero Blanco, Celia

- **MEC-MICINN, Programa Excelencia, FIS2016-79464-P**
  Transporte electrónico, térmico, y de espín con la teoría de funcionales de densidad
  PI: Rubio Secades, Ángel

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia), 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

- **MEC-MICINN, Retos Colaboración, 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

- **CSIC, I-LINK+ 2015**
  Interface processes in layered organic donor-acceptor architectures
  PI: Schiller, Frederik Michael

EUROPEAN AND INTERNATIONAL PROJECTS AND NETWORKS

- **Marie-Curie Action: "Career Integration Grants" (FP7-PEOPLE-2011-CIG), GA 303602**
  MagnetoOrbital - Magnetoelectric couplings in solids and related phenomena
  Supervisor: Souza, Ivo

- **FET Proactive: Atomic and Molecular Scale Devices and Systems (FP7-ICT-2013.9.7), GA 610446**
  PAMS - Planar Atomic and Molecular Scale devices
  PI: Sánchez Portal, Daniel

- **Marie Curie Fellowship (H2020-MSCA-IF-2014), GA 660231**
  SpinMan - Electrical Spin Manipulation in Atoms and Molecules
  Supervisor: Rubio Secades, Ángel

- **NMP - Widening materials models (H2020-NMP-2014), GA 646259**
  MOSTOPHOS - Modelling stability of organic phosphorescent light-emitting diodes
  PI: Rubio Secades, Ángel

- **INFRAIA- Integrating and opening existing national and regional research infrastructures of European interest (H2020-INFRAIA-2014-2015), GA 654360**
  NFFA-Europe - Nanoscience Foundries and Fine analysis for Europe
  PI: Rubio Secades, Ángel

- **ERC Advanced Grant (ERC-2015-AdG), GA 694097**
  QSpec-NewMat - Quantum Spectroscopy: exploring new states of matter out of equilibrium
  PI: Rubio Secades, Ángel

- **Marie Curie Fellowship (H2020-MSCA-IF-2015), GA 702406**
  CoEND - Correlated Electron-Nuclear Dynamics: A novel mixed quantum-semiclassical approach
  Supervisor: Rubio Secades, Ángel

- **Marie Curie Fellowship (H2020-MSCA-IF-2015), GA 704218**
  AMO-dance - Strong Field Dynamics of Atoms and Molecules: History-dependent Functionals and Exact Kohn-Sham Potentials of the Time-dependent (multi-component) Density Functional Theory
  Supervisor: Rubio Secades, Ángel

- **Marie Curie Fellowship (H2020-MSCA-IF-2015), GA 703195**
  SOCISS - Spin-Orbit Coupling at Interfaces from Spintronics to new Superconducting effects
  Supervisor: Rubio Secades, Ángel

- **Marie Curie Fellowship (H2020-MSCA-IF-2015), GA 706890**
  QFluctTrans - Thermodynamics of Quantum Transport
  Supervisor: Rubio Secades, Ángel

- **Marie Curie Fellowship (H2020-MSCA-IF-2016), GA 748971**
  SUPER2D - Superlattices and proximity effects in 2D materials/ molecules hybrid van der Waals heterostructures
  Supervisor: Rogero Blanco, Celia

- **INFRAIA-Integrating Activities for Advanced Communities (H2020-INFRAIA-2016-1), GA 731019**
  EUSMI - European infrastructure for spectroscopy, scattering and imaging of soft matter
  PI: Alegría Loinaz, Ángel

- **Marie Curie Fellowship (H2020-MSCA-IF-2016), GA 753874**
  exciTitania - Excitonic quasiparticles in Titania
  Supervisor: Rubio Secades, Ángel

- **FET-OPEN – Novel ideas for radically new technologies (H2020-FETOPEN-2016-2017), GA 766864**
  MEMO-Mechanics with Molecules
  PI: Lorente Palacios, Nicolás

- **USA Air Force Office of Scientific Research**
  2D Materials and Devices beyond Graphene Science & Emerging Technology of 2D Atomic Layered Materials and Devices
  PI: Rubio Secades, Ángel

- **FLAG-ERA Joint Transnational Call, JTC 2015**
  Trans2DTMD - Theoretical investigation of electronic transport in functionalized 2D transition metal dichalcogenides
  PI: Rubio Secades, Ángel

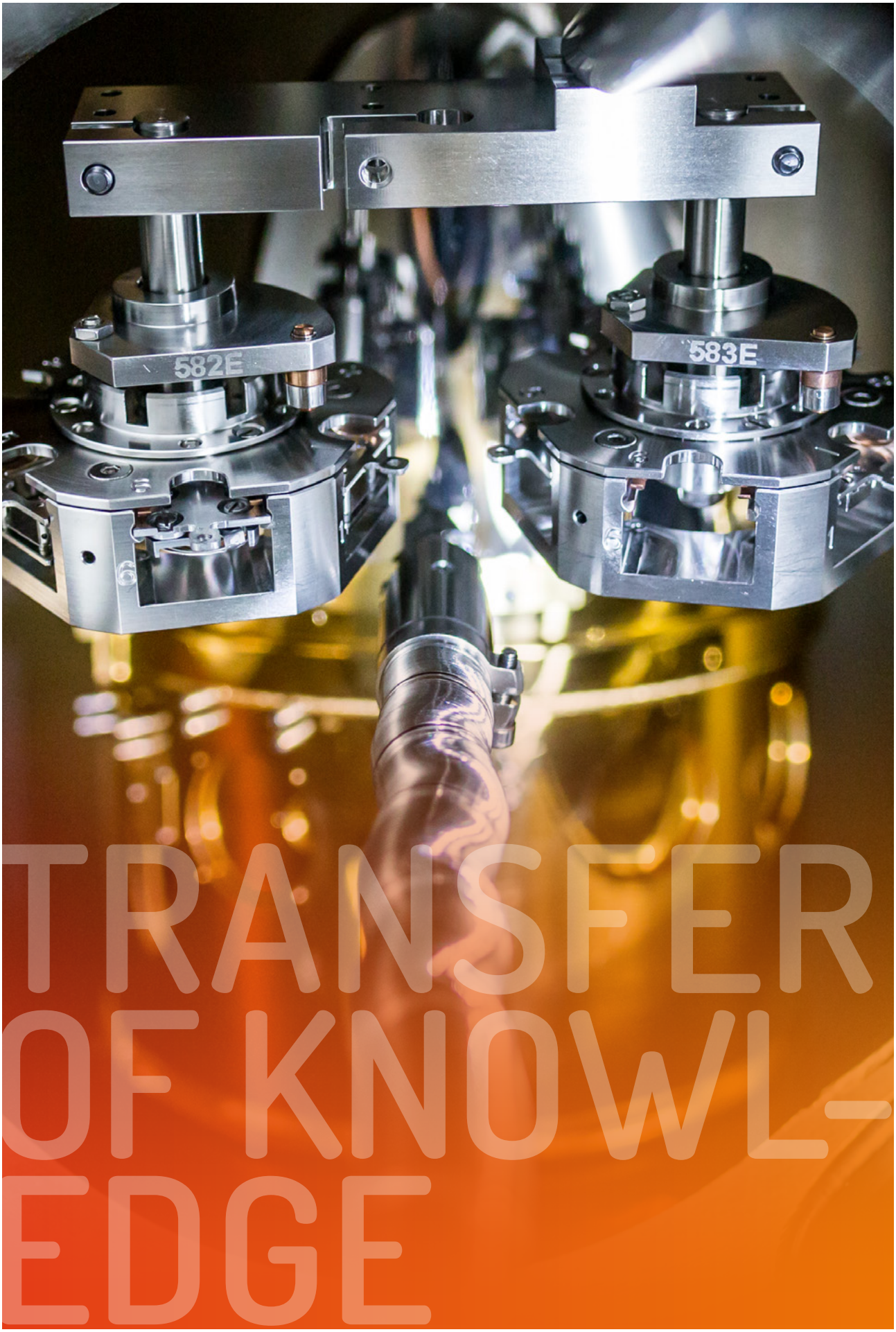
- **COST Action Network, CM1204**
  XLIC: XUV/X-ray light and fast ions for ultrafast chemistry
  PI: Rubio Secades, Ángel

- **COST Action Network, CM1306**
  Modern Tools for Spectroscopy on Advanced Materials: a European Modelling Platform
  PI: Rubio Secades, Ángel

- **COST Action Network, MP1401**
  Advanced fibre laser and coherent source as tools for society, manufacturing and life science
  PI: Fernández Rodríguez, Joaquín

- **COST Action Network, MP1403**
  Nanoscale Quantum Optics
  PI: Aizpurua Iriazabal, Javier

	Funding approved in 2017
BASQUE RESEARCH PROJECTS	333 464 €
SPANISH MINISTRY RESEARCH PROJECTS	185 500 €
EUROPEAN AND INTERNATIONAL PROJECTS AND NETWORKS	994 791 €
MPC-BERC	931 062 €



TRANSFER OF KNOWL-EDGE

TRANSFER OF KNOWLEDGE

In spite of being a fundamental research centre, CFM is committed to give access to all the know how and technologies resulting from its scientific activity in order to have impact on industry and society. A strategy for technology transfer has been developed, generating world-class basic knowledge on advanced materials to be used by local and international private initiatives that involve industrial partners, from large international corporations to SMEs, as well as Technological Centres and CICs.

The portfolio of contracts and collaboration agreements with different companies has been very productive during 2017. Some examples of the partners involved are:

FATE S.A.I.C.I. (Argentina)
'Influence of formulation in the physical properties of vulcanised rubber with silicon and black smoke'

Michelin (France)
'Understanding of plasticizer effect on the temperature dependence of mechanical and dielectric relaxation function of polymers of interest for tire formulation'

FEI Czech Republic S.R.O (Czech Republic)
'Electron microscopy of materials'

Janssen Research (Belgium)
'Study of dielectric properties of polymers'

Basque Culinary Center Fundazioa
'Food science. Physico-Chemical Properties of Complex Materials'

Mugaritz
'Gastronomy and Food Science'

SIMUNE ATOMICS L.T.D.
'Development of software tools to improve the capabilities and the analysis of data computed with the SIESTA/TranSIESTA package'

Považská cementáreň
'Study of hydrated cement pastes'

CFM also tackles strong collaborations devoted to technological transfer towards the Basque Industrial network, within the framework of the ELKARTEK program from the Department of Industry of the Basque Government, as well as towards European Industrial Network (see Research Funding section).

FACILITATING ENTREPRENEURSHIP AND INNOVATION

Enhancing the competitiveness of our local economy and offering new career opportunities to our young researchers is one of the major concerns at CFM. This is the ultimate reason why CFM MPC, in collaboration with BIC Gipuzkoa (an active agent in the support and promotion of entrepreneurial culture in Gipuzkoa), has facilitated the process of creating new businesses based on the scientific developments at CFM, making possible the recruitment of new cohorts of PhDs within the frame of Basque companies and industry. Some of such innovative initiatives are as follows:

BihurCrystal

www.bihurcrystal.com

BihurCrystal provides technology for ultra-high vacuum environments (scientific infrastructure and space applications) and new materials for scientific research. The company employs six Doctors and one technician, all former students at CFM and ICMM *(Instituto de Ciencia Materiales de Madrid).*

Materials Evolution

www.etsf.eu/materials_evolution

Materials Evolution focuses on 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 Ángel Rubio from CFM, and runs in parallel with counterparts in Sweden and Belgium, aiming at providing service over the whole European Region.

Baskrete Energy

Baskrete Energy initiative is a cluster of Basque research and technology centres devoted to launch innovation in the area of cement materials. The network involves a multidisciplinary group of experts from CFM, UPV/EHU, Tecnalia and POLYMAT. Within this network, CFM is focused on the project of exploring the potential of concrete and cement-based materials for energy storage applications.

OUTREACH ACTIVITIES

The role and impact of STEAM (science, technology, engineering, arts and mathematics) has never been as important as it is today. Science has become a key factor directly related to social and economic development. In addition to the importance of sharing the technical scientific output among the scientific community, developing a so called "scientific culture" in the general public has also become crucial in modern societies. In this major task all the members of the scientific community have a role to play, starting from the institutions and including tenured scientists, postdoctoral researchers, PhD students and science communicators. CFM takes full responsibility in science education and communication, as a way to foster a scientifically literate citizenship. The efforts at CFM have been devoted to achieve mainly to objectives: generating scientific vocation and spreading scientific culture to reach broader audiences. Within this spirit, a complete set of scientific outreach activities targeting the general public has been implemented at CFM during 2017. We describe the most important ones below.

HIGH SCHOOL VISITS

Generating scientific vocation is one of the main goals of the outreach strategy at CFM. Since 2013, together with the Donostia International Physics Center (DIPC), CFM has carried out a program of visits where both centres open their doors to high schools students, approximately every two weeks during the academic year.

Besides visiting our facilities, CFM and DIPC offer students the opportunity to directly interact with PhD students, post-doc researchers, professors and other scientific staff, which turns into a unique opportunity for students to learn what research is really about.

During 2017, CFM had the pleasure to host a total of **424** students from **14 schools**, with more than 20 top line researchers involved in this activity. The calendar of visits is displayed as follows:

JANUARY	FEBRUARY	MARCH	APRIL
San Benito Ikastola (Lazkao)	**Summa Aldapeta** (Donostia-San Sebastián)	**Toki Ona BHI (Bera)**	**Laskorain Ikastola** (Tolosa)
Zubiri Manteo Institutua (Donostia-San Sebastián)	**Usandizaga Institutua** (Donostia-San Sebastián)	**Colegio de la Asunción** (Donostia-San Sebastián)	**Koldo Mitxelena BHI** (Errenteria)
MAY	**JULY**	**NOVEMBER**	**DECEMBER**
Facultad Farmacia - Grado de Ciencia y Tecnología de los Alimentos (Vitoria-Gasteiz)	**La Anunciata Ikastetxea** (Donostia-San Sebastián)	**Urola Garaiko Lanbide Eskola** (Zumarraga)	**IES Bidebieta BHI** (Donostia-San Sebastián)
		IES Arrasate BHI (Arrasate)	
		Urola Ikastola BHI (Azpeitia)	

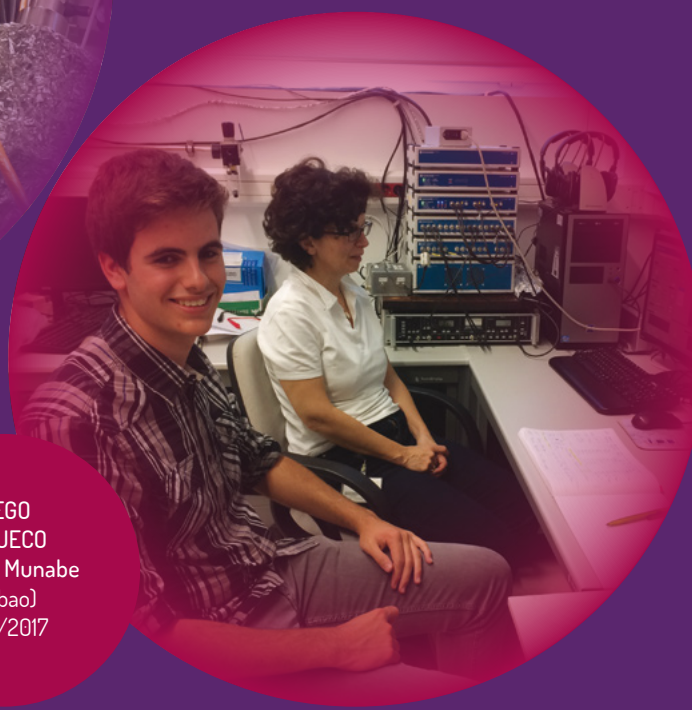
LANALDI PROGRAM

www.lanaldi.es

Lanaldi program, organised by "Fundación Novia Salcedo", provides students a unique opportunity to interact with professionals and share a full day at a scientific centre with them in their working places. This is a great chance for young potential researchers to get a real perspective of the daily life of a scientific research group.

Following the Lanaldi program, during 2017 two students joined the "Spectroscopy at Atomic Scale" group at CFM and shared a day with Lucia Vitali (Ikerbasque Professor and group leader). These are the two students who joined the initiative.

REBECA
URQUIZU RUIZ
Carmelitas Sagrado Corazón
(Vitoria-Gasteiz)
22/2/2017



DIEGO
TAZUECO
Colegio Munabe
(Bilbao)
10/5/2017

XVI SCIENCE WEEK (UPV/EHU)

Tabakalera, Donostia-San Sebastián
8-11 November 2017

From the 8th to the 11th of November of 2017, CFM together with the Donostia International Physics Center (DIPC) and CIC nanoGune, joined the UPV/EHU's week of science with a stand at "Tabakalera" cultural centre in Donostia-San Sebastián. In this stand called **"Inside the Materials World"**, Master and PhD students, as well as post-doctoral researchers of the three centres, got involved in experiments and presentations to show the basis and applications of materials science and other counter-intuitive phenomena to school groups and to the general public.

"A LIFE IN SCIENCE" IN EUREKA! ZIENTZIA MUSEOA

Since 2010, *Eureka! Zientzia Museoa* (the science museum in Donostia-San Sebastián) organises a unique activity, "A life in Science". The event resembles the format of a scientific congress, where active professionals of different scientific disciplines present their "life in science" to high school students with poster sessions and oral contributions. It is a great opportunity for both researchers and students to meet and share experiences and inquiries. CFM supports this successful initiative by sponsoring the meeting as well as actively participating with researchers of different backgrounds of the Centre who share their experiences. More than 300 students and 50 professionals attend the meeting yearly.

In 2017, the following researchers from CFM joined this activity:

- **Edurne Gonzalez** (Fellow Gipuzkoa, CFM)
  Talk: "Nanopartikula disdiratsuak"
- **Daniel E. Martínez-Tong** (Postdoc, DIPC-CFM)
  Talk: "Mi corta pero densa vida científica: de la agronomía a los polímeros"
- **Dimas G. de Oteyza** (Ikerbasque Research Professor, DIPC-CFM)
  Talk: "Física y química de superficies"
- **Paula Malo** (Postdoc, CFM)
  Poster: "La investigación de la materia blanda"
- **Jordan Ochs** (Predoc, DIPC-CFM)
  Poster: "Síntesis y caracterización de poliésteres cíclicos regioregulares"
- **Tineke Van den Berg** (Postdoc, CFM)
  Poster: "Circuit quantum electrodynamics for quantum devices"

"QUÉ SABEMOS DE..." TALK SERIES

Tabakalera, Donostia-San Sebastián
3, 10, 17 and 24 November 2017

Qué sabemos de... is a peculiar series of outreach talks inspired by the intrinsic curiosity of the human being. The program was organised by CFM and CSIC, at the iconic culture centre "Tabakalera" in Donostia-San Sebastián, with the collaboration of *Aulas Kutxa*. More than **400 attendees** participated in the 4 talks organised in this edition of the talks series. The speakers and the topics were as follows:

- **Bernardo Herradón** (CSIC Researcher)
  Talk: "La química una ciencia de cine"
- **Sara Barja** (UPV/EHU Ikerbasque Fellow)
  Talk: "Microscopios: de la célula al átomo"
- **José Luis Fernández Barbón** (CSIC Researcher)
  Talk: "Los agujeros negros y los límites del espacio y el tiempo"
- **Itziar Alkorta** (UPV/EHU Associate Professor)
  Talk: "La carrera armamentística contra las superbacterias. ¿Una lucha desigual?"

See the talks scanning this QR Code

PARTICIPATION IN OUTREACH TALKS

Several outreach talks were given during 2017 by researchers from CFM. We note the following ones:

Reflexiones sobre la identidad
by Gustavo A. Schwartz (Tenured Scientist, CSIC)

Donostidiversity - Asociación Cultural Mestiza,
Palacio de Aiete (Donostia-San Sebastián)
18/11/2017

Cuando los Big Data lo cambian todo
by Gustavo A. Schwartz (Tenured Scientist, CSIC)

Ciclo T+, Casa de América (Madrid)
08/11/2017

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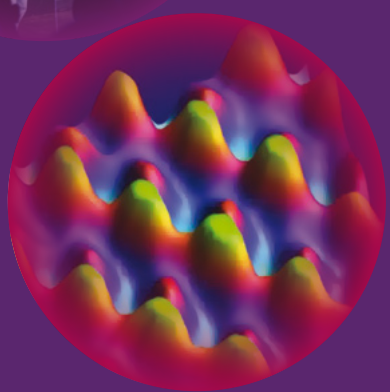


Realidades enredadas y conocimiento transdisciplinar
by Gustavo A. Schwartz (Tenured Scientist, CSIC)

I Jornadas de Investigación Interdisciplinar
(Universidad de Murcia)
30/10/2017

Ciencia de superficie: la vida secreta de las moléculas
by Celia Rogero (Tenured Scientist, CSIC)

Nuevos Caminos de la ciencia, Centro Cultural
Ernest Lluch (Donostia-San Sebastián)
26/10/2017

Comunicación æfectiva de la ciencia
by Gustavo A. Schwartz (Tenured Scientist, CSIC)

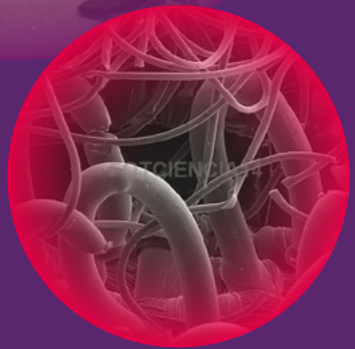
Universidad Pública de Navarra (Pamplona)
11/09/2017

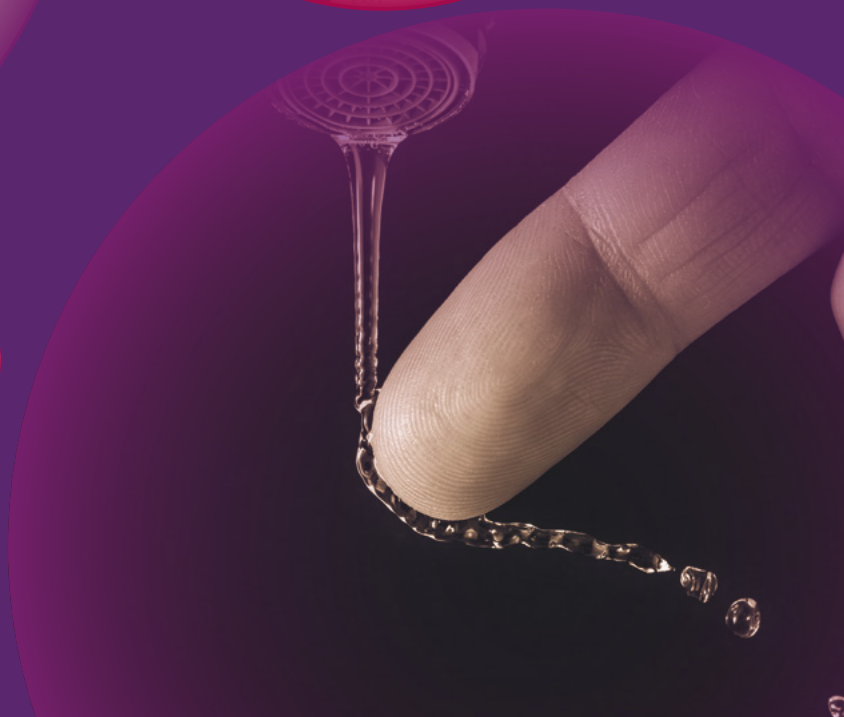
14TH EDITION OF PHOTO EXHIBITION "FOTCIENCIA"

Andrestegi Hall, Carlos Santa Maria centre UPV/EHU
1-29 November 2017

FOTCIENCIA is a photography contest yearly organised by CSIC 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 society inviting researchers as well as citizens to participate in two categories: macro and microscopic photography.

In its 14th edition, from the 700 participating pictures, 49 photographs were selected to be included in this year's exhibition. The set of photographs have been exhibited in several cities around Spain. CFM organised this exhibit in Donostia-San Sebastián, where the amazing set of artistic as well as scientific contributions were visited by a large number of people.





MESTIZAJES

dipc.ehu.es/mestizajes

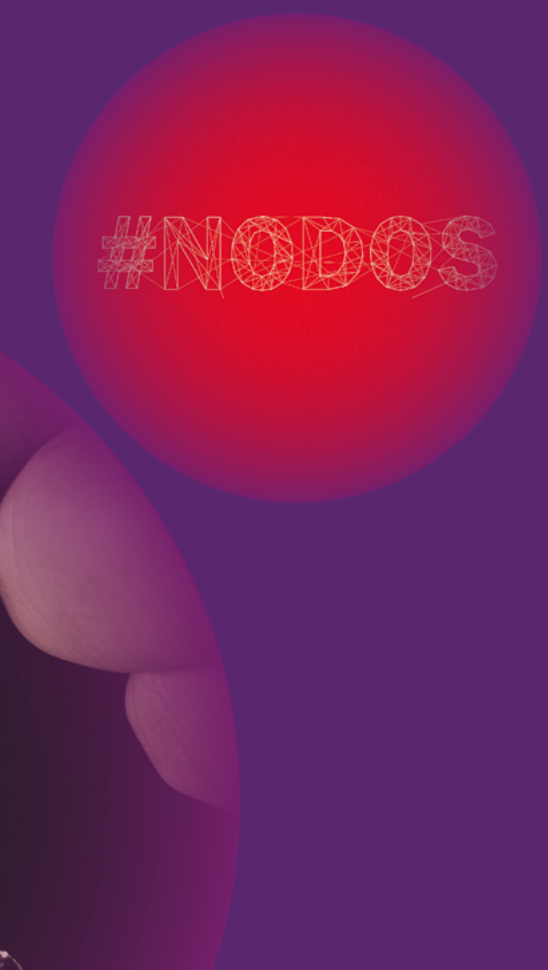
Mestizajes is a programme of the DIPC Foundation which provides an alternative space where scientists, writers, artists and humanists can get together. It is a place for debate, for thinking differently, for giving free rein to the imagination; it's a place for inquiry, for agreement and disagreement; a place for generating and communicating new forms of knowledge. Gustavo Ariel Schwartz, a tenured scientist from CFM, is the founder director of the programme.

International Conference on Literature and Science

Donostia - San Sebastián
23- 25/10/2017

In the frame of the Mestizajes Programme, in October 2017 the III International Conference on Literature and Science was organised: Matter, Life and Consciousness from Science and Literature, gathering an amazing number of invited talks opened to both, specialized and general public.

The aim of this III International Conference was to pursue a journey of 14 billion years of cosmic evolution that has turned matter into life and consciousness. For this, Mestizajes proposes an interdisciplinary perspective that crosses the limits of knowledge between literature and science. Within the meeting, two types of activities were programmed: a workshop aimed at people in the academic field, in the mornings at the DIPC headquarters; and a cycle of open public lectures, in the afternoon at the San Telmo Museum.



Publication of the book #Nodos

Donostia - San Sebastián
16/10/2017

#Nodos is an intellectual adventure that explores the boundaries among different areas of knowledge. #Nodos is a transdisciplinary meeting point where artists, scientists, writers and humanists from different countries share experiences and reflections about the relevance and possibilities of the interaction among different disciplines. It is a book that brings together about 100 contributions from people from different countries from the field of science, humanities, literature and art around ten thematic areas: Complex Networks, Metaphor, Cosmos, Chaos and Complexity, Emergency, Perception, Memory, Emotion, Consciousness and Big data. The edition of the book has been coordinated by Gustavo Ariel Schwartz, tenured scientist from CFM, and Víctor Bermúdez, and it is an excellent example of a transdisciplinary research space. The book has been published by Next Door Publishers and is available in bookstores and on-line. The first edition of the book was sold out in three months. The English version of the book is expected to be published along 2018.

ACTIVITY IN MASS MEDIA

During 2017 CFM was cited over 130 times in the media, including press, online articles, TV and Radio. This activity can be summarized as follows:

Press articles
36

Online press
76

Radio
15

TV
2

The most relevant records can be seen scanning the following code:

An example of this intense activity is the collaboration with the well-known science outreach radio program "La mecánica del caracol", in Radio Euskadi (EITB), performed on a monthly base. Science and particularly Material Physics Science, is presented in a simple and close language, in an effort to make scientific concepts and properties understandable and attractive to the general public. 12 collaborations were recorded in 2017 by CFM's outreach specialist, Idoia Mugica. Following the same collaboration pattern, several programs in "Norteko Ferrokarrila" in Euskadi Irratia (EITB) promoted by Elhuyar fundazioa were recorded in 2017.

OUTREACH COLLABORATION NETWORK

The Center for Materials Physics has established strategic alliances regarding scientific outreach initiatives which create important synergies. These are the main strategic partners of CFM in this strategy:

Universidad del País Vasco/ Euskal Herriko Unibertsitatea

Consejo Superior de Investigaciones Científicas

Donostia International Physics Centre

CIC nanoGUNE

Diputación de Guipuzkoa- Gipuzkoako Foru aldundia

IK4- TEKNIKER

Norteko Ferrokarrila (Elhuyar)

La mecánica del caracol (Radio Euskadi)

Aulas kutxa- kutxakultur

Eureka! Zientzia museoa

HPC Now!

Addlink

Pint of Science

FECYT

Fundación Novia Salcedo

Mestiza (Asociación Artística Sociocultural)

ADDITIONAL COLLABORATIONS

Cátedra de Cultura Ciéntífica (UPV/EHU)

Berritzegune Nagusia (Gob. Vasco)

Asociación Española de Comunicación Científica

Día internacional de la mujer y la niña en la Ciencia

For Women in Science UNESCO/L´oreal

Inspira project (Universidad de DEUSTO, Innobasque and Elhuyar fundazioa)

AWARDS & RECOGNI-TIONS

AWARDS AND RECOGNITIONS

WALTER HÄLG PRIZE

Prof. Juan Colmenero de León

The European Neutron Scattering Association (ENSA) awarded the 2017 Walter Hälg Prize to Prof. Juan Colmenero, leader of the "Polymers and Soft Matter" group at CFM. The Walter Hälg Prize is awarded biannually to a European scientist for outstanding coherent work in neutron scattering with long-term impact on scientific and/or technical neutron scattering applications; a definition reflecting the professional achievements of the person who wins the Prize.

The scientific committee acknowledged the creation of a pioneering unique and robust scientific methodology based on the combination of neutron scattering with different spectroscopic methods and molecular dynamics (MD) simulations, as an outstanding contribution of Professor Juan Colmenero in the field of neutron scattering on complex materials such as polymers or soft matter. Prof. Colmenero was one of the first researchers to recognize that, in intricate soft matter systems, often neutrons alone are not enough to reveal “where the atoms are and what they do”, and that neutron scattering and MD simulations are natural and valuable partners in interrogating matter.

THESIS AWARD

Dr. Ana Belén Sánchez Sánchez

The postgraduate committee of the University of The Basque Country (UPV/EHU) awarded Dr. Ana Belén Sánchez Sánchez the 2017 Extraordinary Doctoral Award for her thesis "Assembly & disassembly of bioinspired single-chain polymer nanoparticles", presented in 2014 under the supervision of Professor J. Pomposo from the "Polymers and Soft Matter" group of CFM. This is the maximum recognition given by the UPV/EHU within a specific area of knowledge.

HIGHLY CITED RESEARCHER

Prof. Javier Aizpurua Iriazabal

Clarivate Analytics has recognised the head of the "Theory of Nanophotonics" group at CFM and DIPC in Donostia-San Sebastián, Prof. Javier Aizpurua, as a highly cited researcher 2017, based on the highly cited papers from 2005 to 2015. Highly-cited researchers are acknowledged by the number of highly-cited papers (in the top 1%) within an area (in this case Physics), according to the database of "Web of Science" over the last eleven-year period. Prof. Javier Aizpurua is one of the five physicists working in Spain, and one of the two researchers in the Basque Country, who have been acknowledged with this recognition.

THE ELEMENTS

OF CFM

cfm.ehu.es

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CFM

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Universidad del País Vasco
Euskal Herriko Unibertsitatea

MPC-BERC
Materials Physics Center
Basque Excellence Research Centre