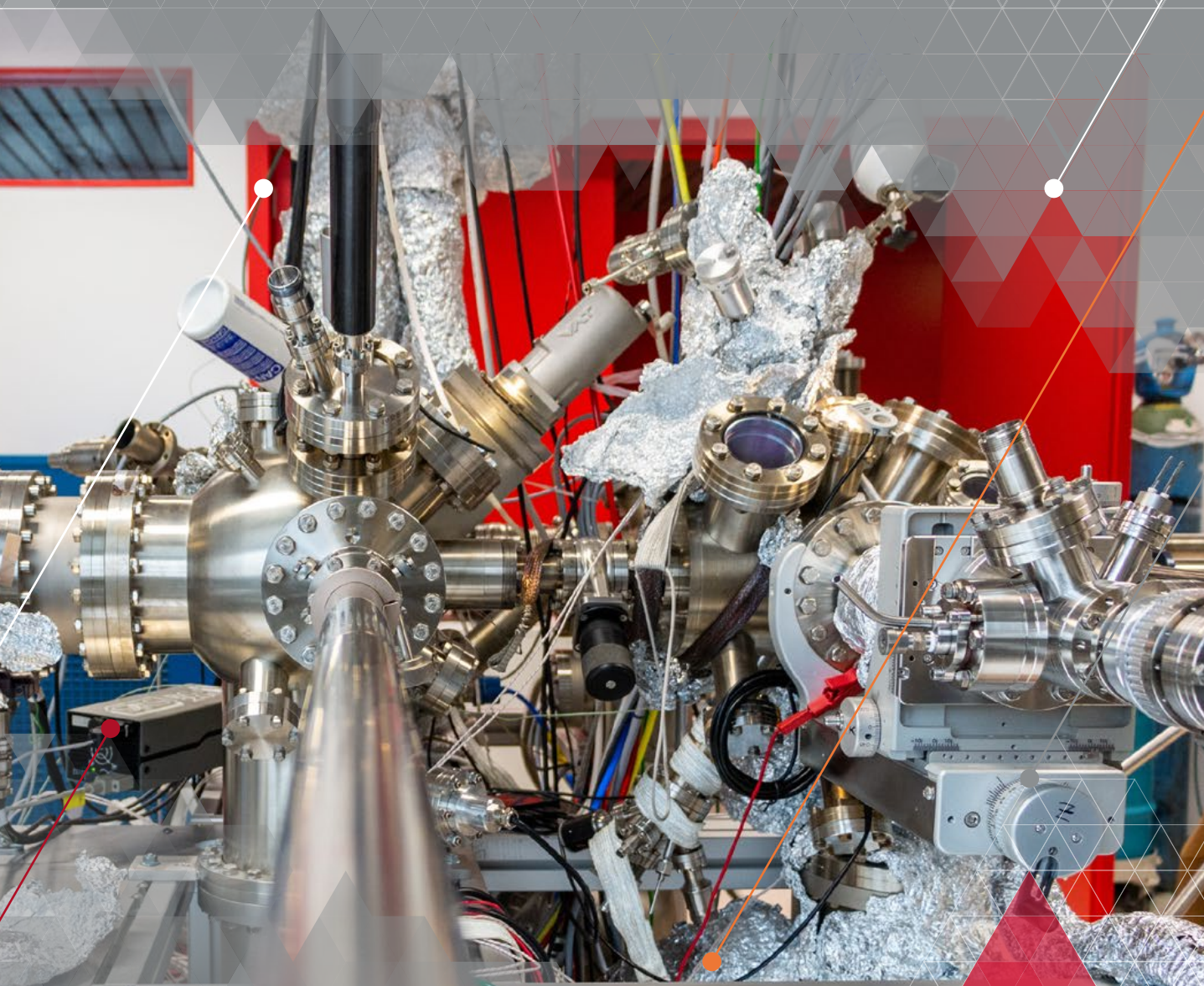
Materialen Fisika Zentroa
Centro de Física de Materiales
Materials Physics Center



ACTIVITY REPORT 2018

CSIC
Consejo Superior de Investigaciones Científicas

Universidad del País Vasco
Euskal Herriko Unibertsitatea

MPC-BERC

ACTIVITY REPORT 2018

CFM

Centro de Física de Materiales

Materialen Fisika Zentroa

Materials Physics Center

CSIC
Consejo Superior de Investigaciones Científicas

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Universidad del País Vasco
Euskal Herriko Unibertsitatea

MPC-BERC
Materials Physics Center
Basic Excellence Research Centre

SUMMARY

FOREWORD

Andrés Arnau Pino, Vicedirector

Javier Aizpurua Iriazabal, Director

One of the main objectives of our community is to develop excellent science while keeping our joy and ethics as fundamental ingredients of our daily tasks. We all put our little brick on the big wall with every contribution we provide in different ways, and each and every one of those contributions is necessary to achieve a better research center and scientific community.

The year 2018 has been a really good one for CFM in many senses. Two new research groups were formally created in the center: the "Quantum Nanophotonics Laboratory", led by Gabriel Molina Terriza, an Ikerbasque Professor, and the "Ceramic and Cement-Based Materials" group led by Jorge Sánchez Dolado, a CSIC tenured scientist. Both groups have extended the current expertise and capabilities at CFM, providing complementary and novel topics to our focus on the Physics of Materials. A third researcher, Ion Errea Lope, an associate lecturer at UPV/EHU, has also joined our center permanently, bringing his expertise in ab-initio calculations of strongly correlated systems to CFM, together with his ERC starting grant. Finally, we are also glad that Vitaly Golovach, an Ikerbasque Fellow, got promoted to Ikerbasque Research Associate, also joining the scientific board of the center. The origins of these four researchers are a good example of the strategic alliance between Ikerbasque, CSIC, and UPV/EHU, which allows our research center to be a better and more competitive one. We would like to welcome the four permanent researchers to our community and wish them all the best among us.

We would also like to pay tribute to another researcher who got retired during 2018. Joaquín Fernández, member of our scientific board, and Professor of the UPV/EHU at the School of Engineering of Bilbao, was one of the founders of the joint CSIC-UPV/EHU unit of Materials Physics in 1999, and his contribution has been always loyal, productive and generous to CFM. Joaquín left CFM during 2018 after he got formal retirement at UPV/EHU, but he will be around, allowing us to enjoy his advice and experience. Thank you Joaquín.

We are at the forefront of the Basque scientific output in Materials Science. Every single contribution matters, and we all are part of this success

Together with the group of permanent researchers, we are fortunate to have 2 research fellows, around 44 postdoctoral researchers and another 51 PhD students in the center. Their effort and commitment is really remarkable and clearly translates into one of the keys of the success at CFM. We are particularly indebted to the transversal and joyful atmosphere created among the students and postdocs from different groups, an extremely positive asset that we do not take for granted.

A new administration manager, Alberto Sainz de Murieta, also joined our center during 2018. We are really happy to have Alberto close to us in order to make crucial decisions regarding financial and human resources in the center. Together with Alberto, everybody working in administration and activity managers have helped us dramatically to conduct all our paperwork and administrative duties in a timely and correct manner. We are really thankful for their attitude and response every time, being aware that they are as important as anybody else to keep the ship sailing at full speed.

The year 2018 has been a good year for CFM in terms of scientific production. More than 175 indexed publications, 65 ongoing research projects (several of them European and international ones), with more than 3.7 million € granted to CFM researchers only in 2018, 10 PhD theses defended, and more than 50 scientific events, such as seminars, workshops, conferences and outreach activities have taken place at CFM. All together, this activity has put ourselves at the forefront of the Basque scientific output in Materials Science. Every single contribution matters, and we all are part of this success.

We are also proud to have launched an important initiative at CFM during 2018. Many of us are aware of the importance of gender equality in all aspects of life and society. Even if real and practical gender equality is a big enterprise and currently a challenge, we have decided to take an explicit step forward to this regard also at CFM by launching the first Gender Equality Plan in the center. The design of this plan started in 2018 and will be completed along 2019, with lots of good proposals and initiatives. Awareness is the first step towards real equality, and we want to be really aware at CFM.

The challenges of a global world are out there, also for a basic research center, which competes with the best centers in the world by developing cutting-edge research on Materials Science. To achieve international recognition in excellent science from a local pole of materials like ours is a big challenge and a joint enterprise. On top of the daily individual effort from all of us, our three key institutions, CSIC, UPV/EHU, and Basque Government, continue their support to our center in many different ways. We are proud to have these three allies completely aligned with us and supportive to our strategic roadmap. The fourth key supporter is our Gipuzkoa Province Government, who has strongly backed up the center's activities with specific competitive grants. We are thankful to the four of them, and encouraged to continue our activity with confidence and enthusiasm in the next years.

Thank you all for your commitment and support,

Even if real and practical gender equality is a big enterprise and currently a challenge, we have decided to take an explicit step forward to this regard

Javier Aizpurua and Andrés Arnau
Director and Vicedirector of CFM

GOVERNANCE

CFM

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

CURRENT DIRECTION BOARD OF CFM

Director: **Javier Aizpurua Iriazabal**

Vicedirector: **Andrés Arnau Pino**

Secretary: **Alberto Sainz de Murieta Álvarez**

SCIENTIFIC BOARD OF CFM

All scientific permanent staff of CFM participates in the Scientific Board. The board is thus made of UPV/EHU staff, CSIC staff, as well as Ikerbasque staff.

CFM

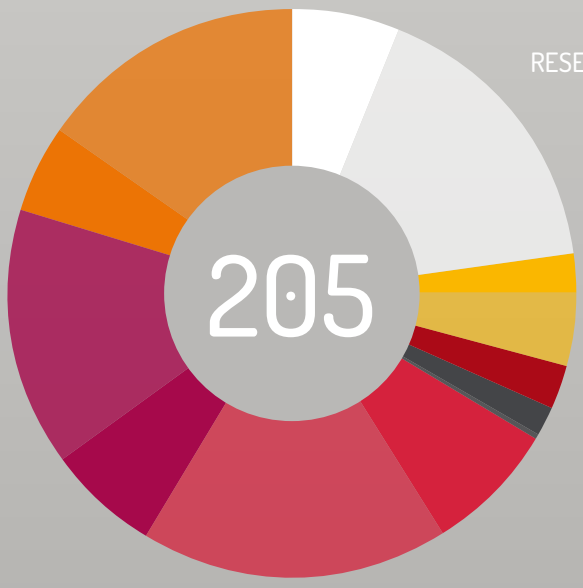
MPC-BERC

The association "Materials Physics Center" (MPC) is a non-profit association declared as Basic Excellence Research Center (BERC) which is intrinsically united to CFM, and shares its goals and scientific activity, serving as an instrumental body in a totally synergistic and combined activity. The body of governance of the MPC-BERC is constituted by the Basque Government (GV), the Gipuzkoa's 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.

MPC - BERC

PROFILE

Researchers in action



46 GUEST RESEARCHERS ♀ ♂

41 PERMANENT RESEARCHERS ♀ ♂

13 UNDERGRADUATE STUDENTS
5 Scholarships ♀ ♂

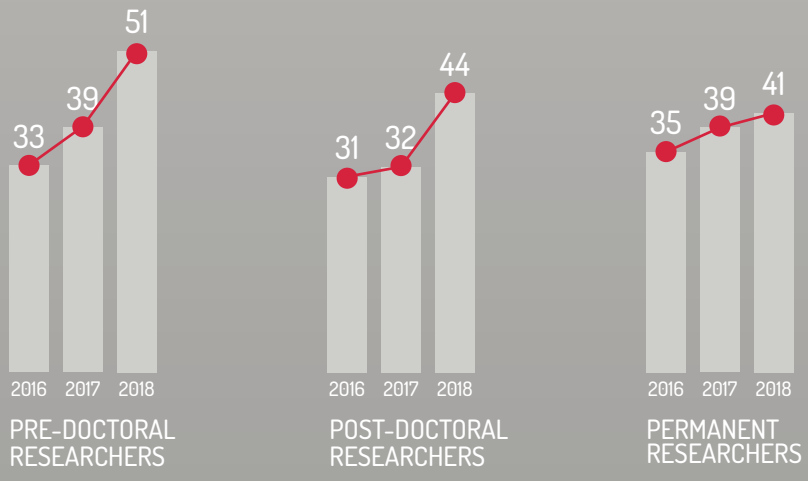
5 MASTER STUDENTS ♂

44 POST-DOCTORAL RESEARCHERS
4 Ikerbasque fellows ♀ ♂

5 TECHNICIANS ♀ ♂

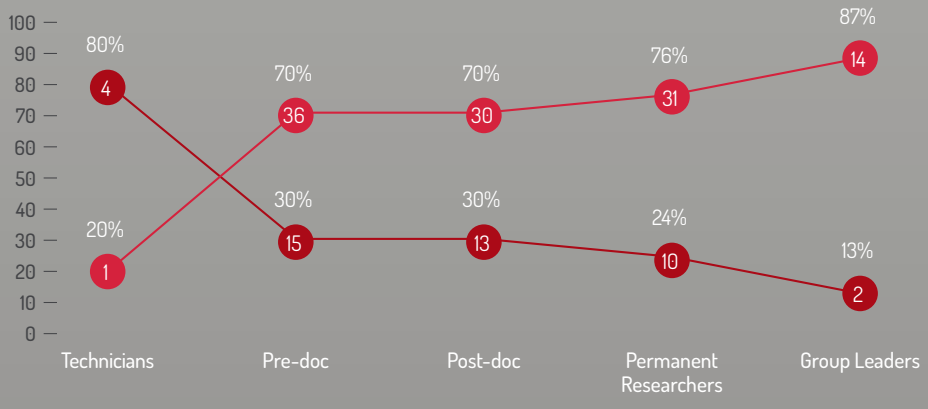
51 PRE-DOCTORAL RESEARCHERS ♀ ♂

Scientific Staff Evolution



Distribution of CFM's Scientific Community by gender

♀ ♂



50% of the Research Community is international

Researchers from other countries **33**

TRAINING

PhD Theses defended **10**

Master Theses defended **8**

Undergrad projects defended **4**

Hosted internships **5**

RESEARCH OUTPUT

ISI Publications **178**

Average impact factor **6.03**

H-index **118**

Q1 Publications **63 %**

Citations* **11191**

* Source: Web of Science Core Collection- CFM's Researcher ID F-4867-2012 as of March 2019

ACTIVITIES AND EVENTS

Seminars **15**

Workshops and conferences **16**

Visitors from Schools **499**

Outreach activities **18**

Impact in the media **148**

PROJECTS AND FUNDING

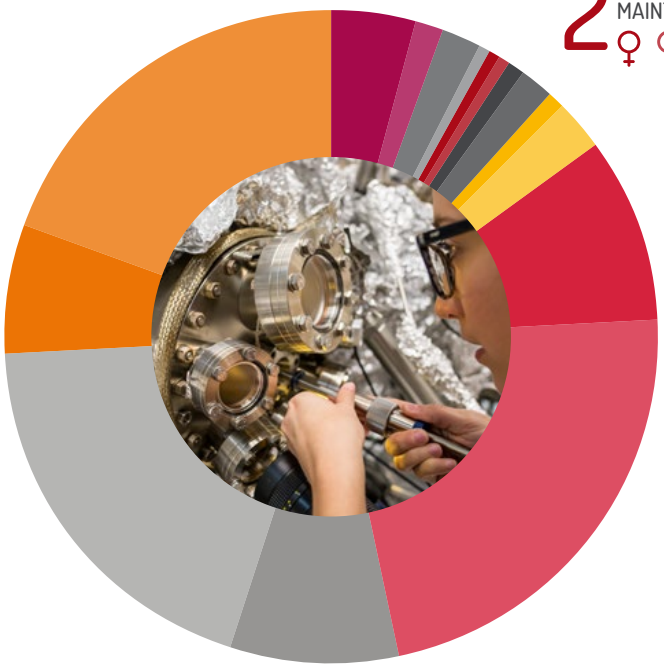
Ongoing projects **65**

Funding 2018 **3 811 580€**

PEOPLE

Distribution of CFM staff during 2018

161



9 ADMINISTRATION AND MANAGEMENT ♀ ♂

5 TECHNICIANS ♀ ♂

2 SERVICES AND MAINTENANCE ♀ ♂

4 COMPUTING SERVICES ♀ ♂

5 UNDERGRADUATE STUDENTS* ♀ ♂

41 PERMANENT RESEARCHERS ♀ ♂

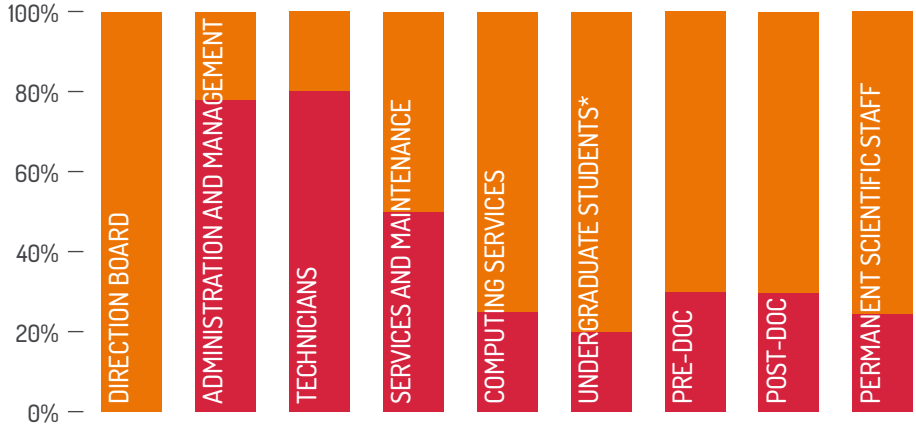
51 PRE-DOCTORAL RESEARCHERS ♀ ♂

44 POST-DOCTORAL RESEARCHERS ♀ ♂

* Only those who received scholarships during their stay at CFM

Staff distribution at CFM according to category and gender

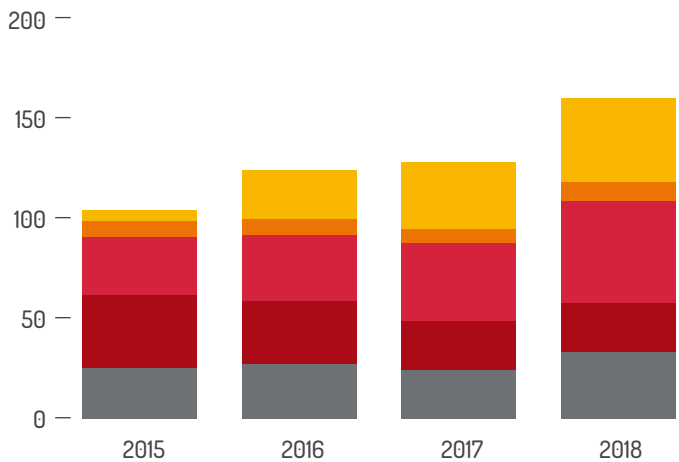
♀ ♂



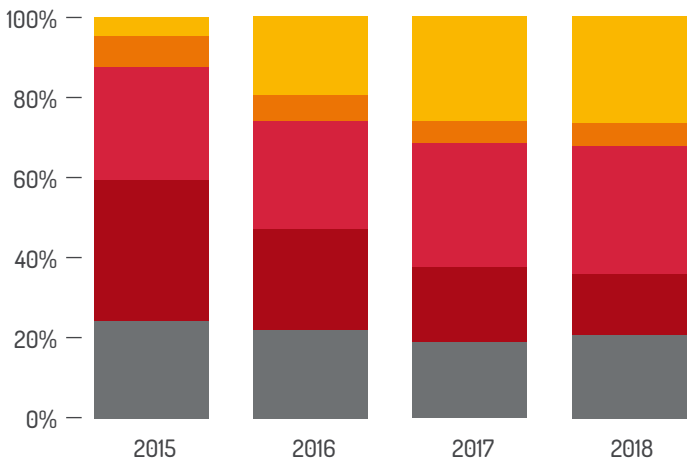
	2015	2016	2017	**2018**
CSIC	25	27	24	**33**
UPV/EHU	36	31	24	**25**
MPC-BERC	29	33	39	**51**
IKERBASQUE	8	8	7	**9**
COLLABORATORS	5	24	33	**43**
Total	103	123	127	**161**

*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.



DIRECTION BOARD

Javier Aizpurua Iriazabal, Director

Andrés Arnau Pino, Vicedirector

Alberto Saínz de Murieta Álvarez, General Manager

ADMINISTRATION AND MANAGEMENT

Alberto Saínz de Murieta Álvarez, Administration Manager, CSIC

Amaya Moral Arce, Administration Manager, CSIC

Ane Iturriza Semperena, Administrative, MPC

Elixabet Sarasketa Zabala, Project and Technology Transfer Manager, MPC

Idoia Mugica Mendiola, Outreach Manager, MPC

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

María Formoso Ferreiro, Administrative, MPC

Marta López Pérez, Administrative, MPC

Txema Ramos Fernández, Administrative, CSIC

COMPUTING SERVICES

Iñigo Aldazabal Mensa, Computer Center Manager, CSIC

Ioritz Paulis Garmendia, IT Systems Technician, MPC

Garbiñe Egaña Cruz, IT Systems Technician, MPC

Reda Hjila, IT Systems Technician, MPC

SERVICES AND MAINTENANCE

Juan Manuel Burgos Jiménez, Maintenance, MPC

Tamara Molina Rolo, Services, MPC

RESEARCHERS

Research Line:

Chemical Physics of Complex Materials

01 Gas/Solid Interfaces

Permanent Researchers

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

Post-doctoral Researchers

Alejandro Rivero Santamaria
Natalia Koval

Pre-doctoral Researchers

Auguste Tetenoire
Alejandro Peña Torres

Guest Researchers

Oihana Galparsoro Larraza, Post-doctoral Researcher
Dino Novko, Post-doctoral Researcher
Ivor Lončarić, Post-doctoral Researcher

02 Quantum Phenomena on Surfaces

Permanent Researchers

Nicolás Lorente Palacios, Scientific Researcher, CSIC

Ikerbasque Fellow

Deung-Jang Choi, MPC

Post-doctoral Researchers

Vladimir Zobac
Roberto Robles Rodríguez

Pre-doctoral Researchers

Cristina Mier González
José Reina Gálvez

Guest Researchers

Young Rok Jang, Scientific Senior
Paula Abufager, Scientific Senior
Fabio Donati, Scientific Senior
Richard Korytár, Scientific Senior
Christoph Wolf, Post-doctoral Researcher
Fernando Delgado Acosta, Post-doctoral Researcher

03 Nanophysics Lab

Permanent Researchers

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

Ikerbasque Fellow

Sara Barja Martínez, UPV/EHU

Post-doctoral Researchers

Andrew Weber
Khadiza Ali
Laura Fernández Gómez-Recuero
Marco Gobbi
Maxim Ilin
Zakaria Abd-El Fattah

Pre-doctoral Researchers

Fernando García Martínez
Carmen González Orellana
Javier Zaldívar Fernández
Marina Peña Díaz
Rishav Harsh
Rodrigo Castrillo Bodero

Master Student

José Enrique Barranco Riveros

Undergraduate Students

Ander Arregui Biera
Ane Telleria Lazcano
Celia González Sánchez
Guillermo Hijano Mendizabal
Irati Garmendia San Miguel

Guest Researchers

Afaf El-Sayed, Scientific Senior
Guy Le Lay, Scientific Senior
Jingcheng Li, Post-doctoral Researcher
Marcos Paradinas Aranjuelo, Post-doctoral Researcher
Kim Akius, Pre-doctoral Researcher
Rishav Harsh, Pre-doctoral Researcher
Roberto Constantini, Pre-doctoral Researcher

04 Modelisation and Simulation

Permanent Researchers

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

Post-doctoral Researchers

Giuseppe Foti
Joseba Alberdi Rodríguez
Mikhail Otrokov
Pablo López Tarifa

Pre-doctoral Researchers

Moritz Müeller
Sophie Espert
Joseba Goikoetxea Perez
Masoud Mansouri
Iker Gallardo Arrieta
Marc Barbry

Guest Researcher

Pavel Jelinek, Scientific Senior

05 Spectroscopy at Atomic Scale

Staff

Lucia Vitali, Ikerbasque Professor, UPV/EHU

Pre-doctoral Researcher

Ana Barragán Durán

Research Line:

Electronic Properties at the Nanoscale

06 Electronic Excitations in Surfaces and Nanostructures

Permanent Researchers

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

Post-doctoral Researchers

Marta Pelc
Romain Dupuis
Jhon Wilfer González Salazar
Ilya Nechaev

Pre-doctoral Researchers

Raúl Guerrero Avilés
Mikel Arruabarrena Larrarte

Master Student

Jozef Janovec

Guest Researchers

José Salvador Surga Díez, Scientific Senior
Erik Díaz Cervantes, Post-doctoral Researcher
Magdalena Marganska, Post-doctoral Researcher

07 Materials Computation and Theory

Permanent Researchers

Aitor Bergara Jauregi, Associated Professor, UPV/EHU
Ion Errea Lope, Associate Professor, UPV/EHU
José María Pitarke de la Torre, University Professor, UPV/EHU

Pre-doctoral Researchers

Iñigo Robredo Magro
Miguel Borinaga Treviño
Oscar Rodríguez Ballesteros
Unai Aseguinolaza Aguirreche

08 Mesoscopic Physics

Permanent Researchers

F. Sebastián Bergeret Sbarbaro, Tenured Scientist, CSIC

Ikerbasque Associate

Vitaly Golovach, UPV/EHU

Post-doctoral Researchers

Tineke van den Berg

Pre-doctoral Researchers

Alba Pascual Gil
Cristina Sanz Fernández
Xianpeng Zhang
Julie Isabelle Baumard
Mikel Rouco Martín

Master Student

Ricardo Rama Eiroa

Undergraduate Student

Alberto Hijano Mendizabal

Guest Researchers

Maxim Kharitonov, Scientific Senior
Miguel Ángel Cazalilla Gutiérrez, Scientific Senior
Chunli Huang, Pre-doctoral Researcher

09 Nano-Bio Spectroscopy

Permanent Researchers

Ángel Rubio Secades, University Professor, UPV/EHU

10 Souza Research Group

Permanent Researchers

Ivo Souza, Ikerbasque Professor, UPV/EHU

Post-doctoral Researchers

Tomas Rauch
Stepan Tsirkin
Julen Ibañez Azpiroz

Pre-doctoral Researcher

Miguel Ángel Jiménez Herrera

Guest Researchers

Cheol-Hwan Park, Scientific Senior
Raffaele Resta, Scientific Senior
Jaemo Lin, Pre-doctoral Researcher

11 Ceramic and Cement-Based Materials

Permanent Researcher

Jorge Sánchez Dolado, Tenured Scientist, CSIC

Post-doctoral Researcher

Guido Goracci

Guest Researcher

Albina Kostiuchenko, Pre-doctoral Researcher

Research Line:

Photonics

12 Theory of Nanophotonics

Permanent Researchers

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

Post-doctoral Researchers

Garikoitz Aguirregabiria Achutegui
Luca Bergamini
Mario Zapata Herrera
Tomas Neuman

Pre-doctoral Researchers

Álvaro Nodar Villa
Andrea Konečná
Antton Babaze Aizpurua
Carlos Maciel Escudero

Undergraduate Student

Unai Arregui León

Guest Researchers

Emily Anne Townsend, Scientific Senior
Garnett Bryant, Scientific Senior
Fani Madzharova, Pre-doctoral Researcher
Rafael Muñoz Mármol, Pre-doctoral Researcher

13 Nanomaterials and Spectroscopy

Permanent Researcher

Yury Rakovich, Ikerbasque Professor, UPV/EHU

Post-doctoral Researcher

Thomas Hendel

Master Student

Semen Goncharov

14 Laser Physics and Photonic Materials

Permanent Researchers

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

15 Quantum Nanophotonics Laboratory

Permanent Researchers

Gabriel Molina Terriza, Ikerbasque Professor, MPC

Post-doctoral Researcher

Juan José Miguel Varga

Pre-doctoral Researchers

Martín Molezuelas Ferreras
Jon Lasa Alonso

Undergraduate Student

Evan Villafranca

Guest researchers

Juliet Gonipath, Permanent Researcher
Reece Roberts, Pre-doctoral Researcher

Research Line:

Polymers and Soft Matter

16 Polymers and Soft Matter

Permanent Researchers

Ángel Moreno Segurado, Tenured Scientist, CSIC
Ángel Alegría Loinaz, University Professor, UPV/EHU
Arantxa Arbe Méndez, Research Professor, CSIC
Daniele Cangialosi, Tenured Scientist, CSIC
Fernando Álvarez González, Associate Professor, UPV/EHU
Gustavo A. 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

Post-doctoral Researchers

Beatriz Robles Hernández
Daniel E. Martínez Tong
Daniel J. Arismendi Arrieta
Edurne Gonzalez Gandara
Guadalupe Natalia Ruiz Tabbia
Izaskun Combarro Palacios
Marina Gonzalez Burgos
Mohammad Ali Aboudzadeh Barihi
Paula Malo de Molina Hernández
Xabier Gaetan Monnier

Pre-doctoral Researchers

Amaia Matanza Corro
Ander Mendia Velasco
Jon Rubio Cervilla
Jordan Ochs
Jorge Melillo
Julen De la Cuesta Leone
Lucia Ortega Álvarez
Maiara Aime Iriarte Alonso
Mariarita Paciolla
Maud Formanek
Natalia Gutiérrez Pérez de Eulate
Thomas Louis Gambino

Scientific Technicians

Amaia Iturrospe Ibarra, MPC
Luis Botana Salgueiros, CSIC
María Isabel Asenjo Sanz, MPC
María Lourdes Leza Fernández, UPV/EHU
Silvia Arrese-Igor Irigoyen, CSIC

Master Student

Javier Martínez Sabando

Undergraduate Students

Jokin Pinacho Olaciregui
Julen Gorospe Trujillo
Nidybeth Tatiana Claros Gutiérrez

Guest Researchers

Carmen Mijangos Ugarte, Scientific Senior
Erik B. Berda, Scientific Senior
Jozef Bartos, Scientific Senior
Julian Oberdisse, Scientific Senior
Nadia Lotti, Scientific Senior
Helena Svajdlenkova, Post-doctoral Researcher
Michelina Soccio, Post-doctoral Researcher
Murillo Longo Martins, Post-doctoral Researcher
Hamidreza Heydarnezhad, Pre-doctoral Researcher
Paul Markus, Pre-doctoral Researcher

OTHER POSITIONS

Associate Professors

Isabel Tellería Echeverría, UPV/EHU

Scientific Researchers

Fabienne Barroso Bujans, Ikerbasque Research Professor, DIPC
Dimas García de Oteyza, Ikerbasque Research Professor, DIPC
Miguel Moreno Ugeda, Ikerbasque Research Associate, DIPC

Post-doctoral Researchers

Luciano Colazzo, DIPC (Dimas García de Oteyza's group)
James Lawrence, DIPC (Dimas García de Oteyza's group)

Pre-doctoral Researchers

Paul Lukas Dreher, DIPC (Miguel Moreno Ugeda's group)
Alejandro Berdonces Layunta, DIPC (Dimas García de Oteyza's group)
Néstor Merino Díez, DIPC (Dimas García de Oteyza's group)
Mohammed Sabri Gamal Mohammed, DIPC (Dimas García de Oteyza's group)

Undergraduate Students

Mikel Dolz, DIPC (Fabienne Barroso Bujans's group)
Pedro Liz Basteiro, DIPC (Fabienne Barroso Bujans's group)

Guest Researchers

María Ángeles Hernández Vozmediano, Scientific Senior
Wen Wan, Pre-doctoral Researcher (Miguel Moreno Ugeda's group)
Julio Alonso Martín, University Professor

EXTERNAL ADVISORY COMMITTEE

Professor Antonio Hernando Grande

Universidad Complutense de Madrid, Spain

Expertise in the line of Electronic Properties at the Nanoscale

Honors and Awards

Director of *Instituto de Magnetismo Aplicado (IMA); Académico Numerario de la Real Academia de Ciencias Exactas, Físicas y Naturales;* Honoris Causa Doctor by the UPV/EHU and by the Cantabria university; 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.

Research Interests

Magnetism and related areas. He combines basic research of magnetic materials with projects in applied research.

Professor Peter Saalfrank

Institut für Chemie, Universität Potsdam, Germany

Expertise in the line of Chemical Physics of Complex Materials

Honors and Awards

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

Professor Dieter Richter

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

Expertise in the line of Polymers and Soft Matter

Honors and Awards

Director of the Institute for Neutron Scattering at the FZJ (1989-2014); Chair at the Materials Physics Department of the University of the Basque Country founded by the Bank of Bilbao Vizcaya (1997); *"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.

Professor Francisco J. García Vidal

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

Expertise in the line of Photonics

Honors and Awards

Director of the IFIMAC- Condensed Matter Physics Center (*María de Maeztu* Center); 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 of Science, Innovation and Universities.

Research Interests

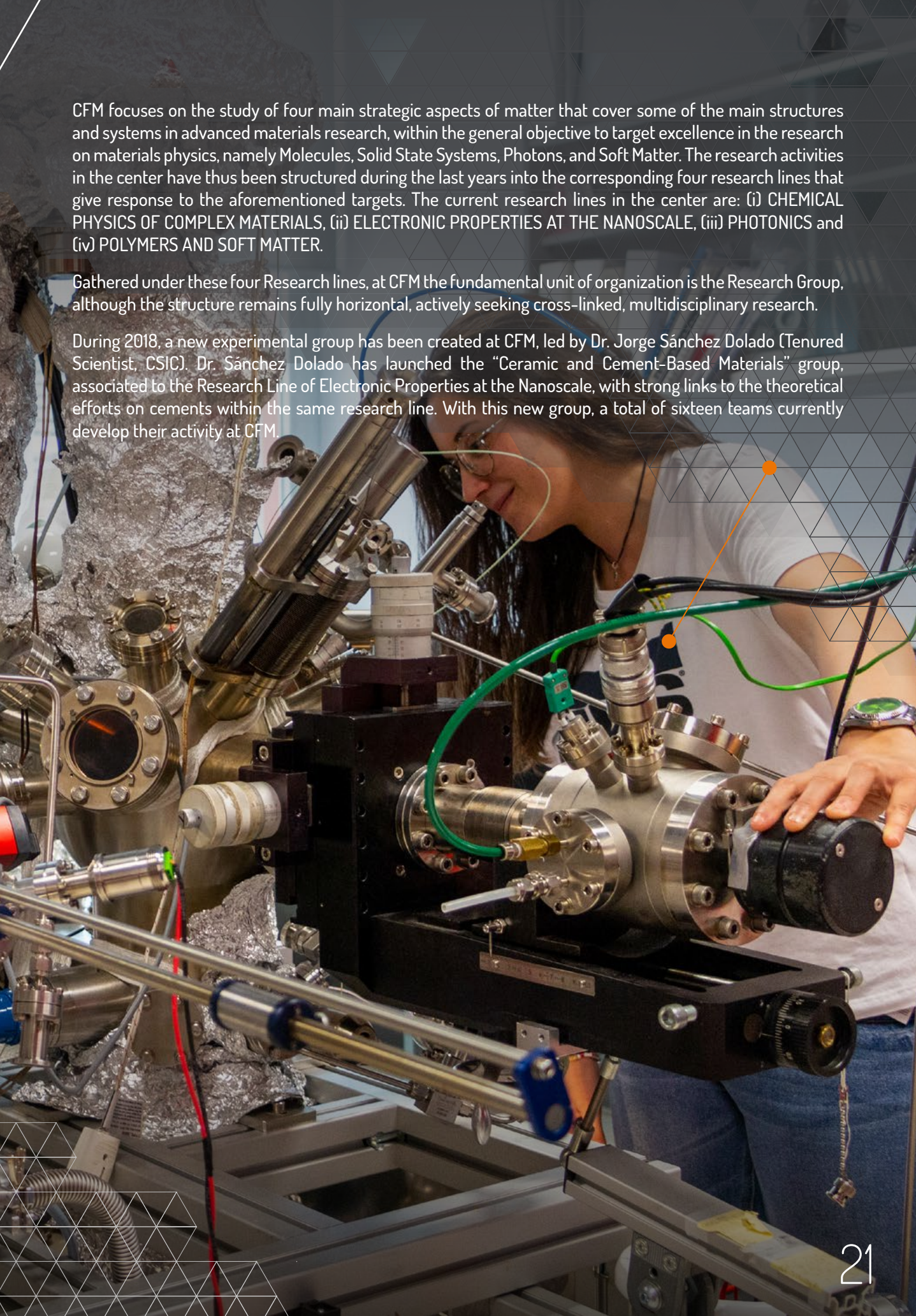
Photonics and nanophotonics.

RESEARCH LINES, GROUPS & HIGHLIGHTS

CFM focuses on the study of four main strategic aspects of matter that cover some of the main structures and systems in advanced materials research, within the general objective to target excellence in the research on materials physics, namely Molecules, Solid State Systems, Photons, and Soft Matter. The research activities in the center 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 center are: (i) CHEMICAL PHYSICS OF COMPLEX MATERIALS, (ii) ELECTRONIC PROPERTIES AT THE NANOSCALE, (iii) PHOTONICS and (iv) POLYMERS AND SOFT MATTER.

Gathered under these four Research lines, at CFM the fundamental unit of organization is the Research Group, although the structure remains fully horizontal, actively seeking cross-linked, multidisciplinary research.

During 2018, a new experimental group has been created at CFM, led by Dr. Jorge Sánchez Dolado (Tenured Scientist, CSIC). Dr. Sánchez Dolado has launched the "Ceramic and Cement-Based Materials" group, associated to the Research Line of Electronic Properties at the Nanoscale, with strong links to the theoretical efforts on cements within the same research line. With this new group, a total of sixteen teams currently develop their activity at CFM.

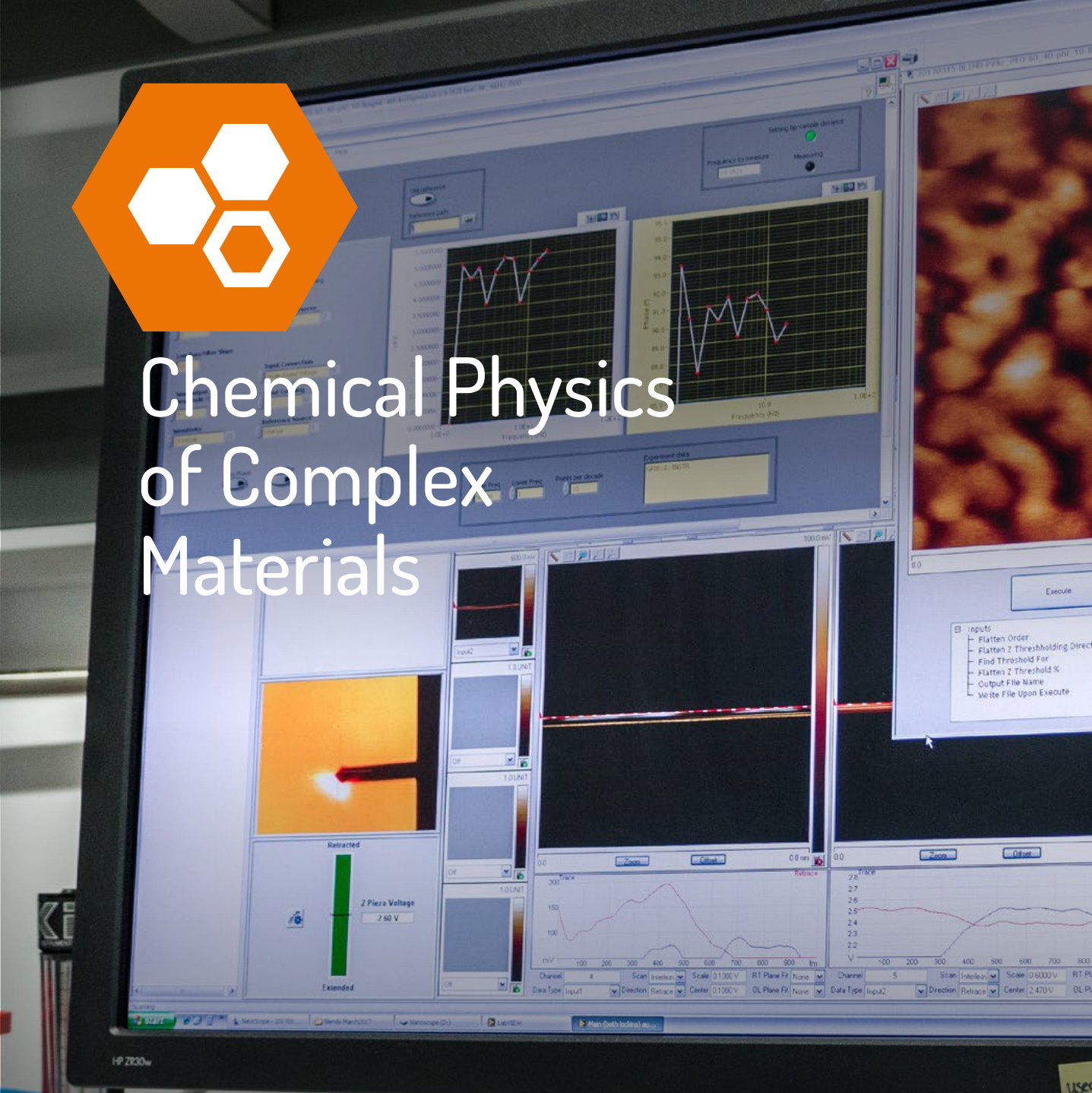


RESEARCH LINES, GROUPS AND HIGHLIGHTS

RESEARCH LINE	GROUP	PROFILE
Chemical Physics of Complex Materials	01 Gas/Solid Interfaces	Theoretical
	02 Quantum Phenomena on Surfaces	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 Souza Research Group	Theoretical
	11 Ceramic and Cement-Based Materials	Experimental
Photonics	12 Theory of Nanophotonics	Theoretical
	13 Nanomaterials and Spectroscopy	Experimental
	14 Laser Physics and Photonic Materials	Experimental
	15 Quantum Nanophotonics Laboratory	Experimental
Polymers and Soft Matter	16 Polymers and Soft Matter	Theoretical and Experimental

Fourteen of these 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), 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 "Quantum Phenomena on Surfaces Group". The other two groups in this research line develop experimental activity on the electronic properties of molecules and low dimensional structures, which are experimentally studied with the use of Scanning Tunneling Microscopy (STM) at ultrahigh vacuum and low temperature, together with a combination of Surface Physics techniques. These are the "Nanophysics Laboratory" and the "Spectroscopy at Atomic Scale" groups.

In what follows, some aspects of the activity of the five research groups included in this research line are described.

Group Leader:
Ricardo Díez
Muiño, Scientific
Researcher, CSIC

01 Gas/Solid Interfaces

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

Electron-mediated phonon-phonon coupling drives the vibrational relaxation of molecules at metal surfaces

Novko D, Alducin M, and Juaristi JI.

Physical Review Letters 120, 156804 (2018)

Novko et al. bring forth a consistent theory for the electron-mediated vibrational intermode coupling that clarifies the microscopic mechanism behind the vibrational relaxation of adsorbates on metal surfaces. This analysis points out the inability of state-of-the-art nonadiabatic theories to quantitatively reproduce the experimental linewidth of the CO internal stretch mode on Cu(100) and it emphasizes the crucial role of the electron-mediated phonon-phonon coupling in this regard. The results demonstrate a strong electron-mediated coupling between the internal stretch and low-energy CO modes, but also a significant role of surface motion.

There is no doubt that the efficiency in creating low-energy electronic excitations must be responsible for decreasing the lifetime of vibrationally excited adsorbates from the millisecond scale in semiconductors to the picosecond scale in metals. The absence of an energy threshold for creating electronic excitations in the latter facilitates the vibrating molecule to transfer part of its energy to the substrate by creating electron-hole pairs excitations, irrespective of the value of the energy with which the molecule vibrates. Even if this physical picture is clear and well established, present first principles theories that account for this electron-vibration coupling are still unable to explain the fast vibrational relaxation that is reported experimentally.

In this letter, Novko et al. demonstrate that the electron-mediated intermode vibrational coupling is the missing piece in our understanding of the controversial nonadiabatic vibrational relaxation. Electrons, besides coupling directly to the vibrating molecules, drive the otherwise forbidden coupling between modes with very different energies. It is the combination of these two effective relaxation mechanisms that finally reconcile the theoretical predictions with experiments. Additionally, this study elucidates the underlying cause of the elusive temperature dependence measured in the high-energy mode relaxation rates. Considering that the relaxation rates are fundamental building blocks for the theoretical description of dynamical process at metal surfaces, this new theory will enrich our understanding of nonadiabaticy not only in vibrating adsorbates, but even more generally in many other surface reactions.

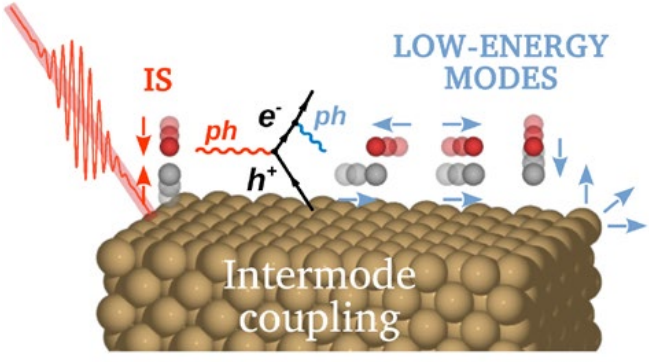


Figure: *Schematic figure of the electron-mediated phonon-phonon coupling process of the internal stretch mode of CO on Cu(100). The internal stretch mode (red) couples to low energy frustrated rotation and frustrated translation modes, as well as to the modes consisting of the joint motion of CO and Cu surface atoms (blue).*

Group Leader: Nicolás Lorente Palacios, Scientific Researcher, CSIC

02

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 STM.

HIGHLIGHT

One step to create topologically non-trivial excitations on superconductors

Choi DJ, García Fernández C, Herrera E, Rubio-Verdú C, Ugeda MM, Guillamón I, Suderow H, Pascual JI, and Lorente N.

Physical Review Letters 120, 167001, 2018

The superconducting gap in the presence of magnetic impurities is weakened and single-electron states can be formed. As the number of impurities increase, the states give rise to bands that can eventually present topological character. This work shows that to create electronic states produced by more than one impurity, the local magnetic moments of the impurity need to align and that the alignment depends on the position of the impurity.

This work presents the first manipulation of individual atoms on the surface of a single crystalline superconducting compound. A superconductor is a metal where the electron-vibration coupling is large enough to create pairs of electrons at low temperature. If all electrons are paired, there are no single-electron conduction channels and it is impossible to inject an electron at low energies. It is well known that magnetic impurities weaken the pairs by creating a local magnetic field that attracts one of the electrons and repels the other electron. In the process of doing so, single-electron states appear at low energies.

In the present contribution, Choi et al., study these single-electron states when two magnetic impurities are at different distance between each other. They show that the induced states in the superconductor reveal a lot of information on the impurities and particularly on their mutual interaction. If the magnetic moments of the impurities are aligned, the local "magnetic field" is enhanced and hybridization of single-electron states is possible with a characteristic signature in the differential conductance. If the magnetic moments are anti-aligned, the single-electron states do not interact and an effect similar to the single-impurity conductance is found. These studies are a step forward in the process of creating quantum states with atomic precision and with control of all the quantum properties of matter.

The work was led by Deung-Jang Choi (Ikerbasque, CFM), and involves researchers from CFM, CIC nanoGUNE, DIPC, and *Universidad Autónoma de Madrid.*

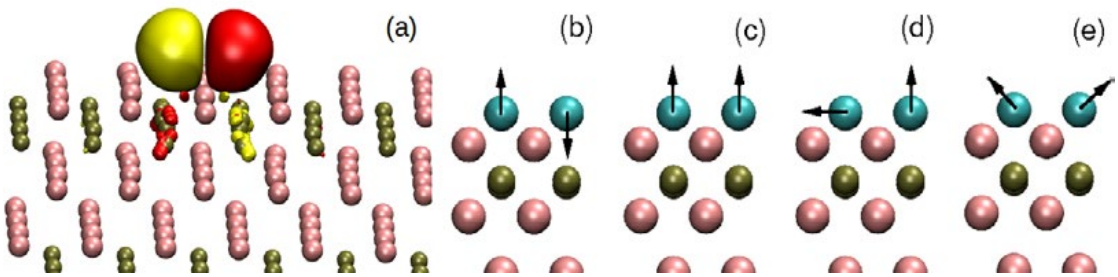


Figure: *Magnetic moment density (a) over a Cr2 dimer on the Bi-rich surface of the superconductor. Yellow is for magnetic moment pointing in the up direction and red in the down direction, corresponding to the antiferromagnetic ordering of figure (b). The other cases are possible magnetic moment orientations on the surface. Spin-orbit coupling is large and non-collinear arrangements are possible although they were not found in the experiment.*

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

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 center 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 characterization 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 characterization 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

Electronic structure tunability by periodic meta-ligand spacing in one-dimensional organic semiconductors

Piquero-Zulaica I, Garcia-Lekue A, Colazzo L, Krug CK, Mohammed MSG, Abd El-Fattah ZM, Michael Gottfried J, de Oteyza DG, Ortega JE, and Lobo-Checa J.

ACS Nano 12, 10537 (2018)

The rapid progress of "on-surface chemistry" has produced a highly versatile bottom-up tool for the controlled-synthesis of atomically precise graphene-based nanostructures. As the resulting polymers are promising candidates for the realization of exotic nanodevices, resolving their electronic structures is key for future technological applications.

In this work, researchers from CFM and DIPC, in collaboration with international partners, have transformed the electronic band structure of the well-known poly-(para-phenylene) (PPP) by introducing periodically spaced meta-junctions into its conductive path. They have achieved the on-surface synthesis of an extended (saturated) polymeric film, which they have macroscopically aligned on a vicinal Ag (111) surface. The atomically precise cross-conjugated oligophenylene zigzag chains host periodically spaced meta-junctions that remain sufficiently decoupled from each other and from the substrate. The experimentally unreported band structure showing weakly dispersing one-dimensional electronic bands along the chain direction, which fully agrees with the theoretical simulations, is presented in this work. A significantly larger frontier orbital band gap than for PPP chains is found, which linearly decreases with the length of the straight segments. Moreover, confinement effects are observed between the elbows of the chains, acting as an array of weakly interacting quantum dots whose localized states can be engineered by increasing the separation between meta-junctions.

These findings corroborate the important effects that the conductive path topology of a molecular wire has on its electronic states, which are responsible for defining its chemical, optical and electronic properties. Such arrays of semiconducting quantum dots hold potential for designing future oligophenylene based quantum devices.

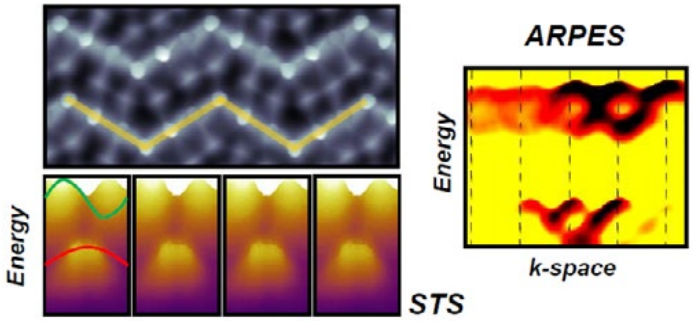


Figure: *Bond-resolution STM image of the zigzag polymer film (top). Bound molecular states localized within the straight segments of the polymer probed by STS (bottom). ARPES electronic band structure of the zigzag polymer chains evidencing shallow dispersive bands (right).*

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 behavior 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 at CFM, and also with groups from other research centers 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 also been 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

Evidence of large spin-orbit coupling effects in quasi-free-standing graphene on Pb/Ir(111)

Otrokov MM, Klimovskikh II, Calleja F, Shikin AM, Vilkov O, Rybkin AG, Estyunin D, Muff S, Dil JH, Vázquez de Parga AL, Miranda R, Ochoa H, Guinea F, Cerdá JI, Chulkov EV, and Arnau A.

2D Mater. 5, 035029 (2018)

Extending graphene's functionalities, beyond those intrinsically inherent to it, aiming at its application in electronic and spintronic devices, has become nowadays a great challenge of contemporary solid state physics. In particular, significant attention is being paid to the enhancement of spin-orbit coupling in graphene, which would enable a number of interesting applications, such as spin Hall effect or its quantum version. In our combined scanning tunneling microscopy, angle- and spin-resolved photoemission spectroscopy and density functional theory study of graphene/Ir(111) intercalated with a Pb monolayer the authors scrutinize and explain the spin-orbit effects induced in graphene by the heavy atoms substrate.

Pb-intercalated graphene on Ir(111) shows a moiré pattern with the same lateral periodicity as graphene/Ir(111). Below graphene, the Pb layer on Ir(111) forms three spatially separated rotational domains in a rectangular structure, commensurate with the Ir(111) lattice. The net result of the Pb monolayer intercalation is that it decouples the carbon sheet from the substrate, resulting in an almost free-standing and perfectly flat graphene overlayer with preserved A–B sublattice symmetry, as observed by low temperature Scanning Tunneling Microscopy (STM). This quasi-free-standing character of graphene on Pb/Ir(111) is further confirmed by both Angle-Resolved Photoemission Spectroscopy (ARPES) measurements and Density Functional Theory (DFT) calculations, both revealing an almost perfectly linear dispersion of the graphene bands and the absence of a gap at the Dirac point.

Despite the apparent decoupling of graphene from the substrate, large spin-orbit (SO) splittings (up to several tens of meV), as well as sizable both in-plane and out-of-plane spin components, arise in graphene bands near the K point of the Brillouin zone, as confirmed by both spin-ARPES measurements and DFT calculations. This non-planar spin texture indicates that both Rashba (extrinsic) and Kane-Mele (intrinsic) SO couplings are induced in graphene. Since no bandgap has been found at the Dirac point, this very fact suggests that the intrinsic contribution to SO interaction does not exceed the extrinsic contribution. The detailed DFT calculations provided by the authors reveal that the intercalated Pb layer does not induce the out-of-plane spin components on its own, contributing only to the Rashba SO coupling in graphene. The origin of the vertical spin components in graphene traces back to the out-of-plane spin-polarized surface and resonance states of the pristine Ir(111) surface. However, the role of the intercalated Pb layer, whose rectangular symmetry imposes the Brillouin zone folding and leads to a closure of the Ir(111) projected bandgap, is instrumental for the linearization of graphene bands. Indeed, due to the band folding induced by the Pb interlayer, most of the Ir(111) surface states are converted into resonances. Therefore, these states become broadened and their hybridization with the graphene bands weakens as compared to graphene/Ir(111), i.e., in the absence of intercalated Pb.

This study appears to be the first to both visualize and explain the Kane-Mele SO coupling contribution to the graphene's Dirac cone spin texture in a real system. The interpretation of the complex spin texture observed in graphene/Pb/Ir(111) has become possible thanks to the state-of-the-art DFT methodology implemented in the SIESTA-GREEN code. This program package allows an efficient treatment of large systems with SO interaction included (the computational cells up to ~900 atoms have been used in the present study) by using a recursive Green function method to treat the semi-infinite medium, as well as an unfolding procedure of the large supercell folded bands. This is the only way in which spin-ARPES data can be compared with the calculated graphene bands, although strictly speaking one should talk, instead of «bands», about wave-vector-, energy-, and layer-resolved densities of states or spin densities.

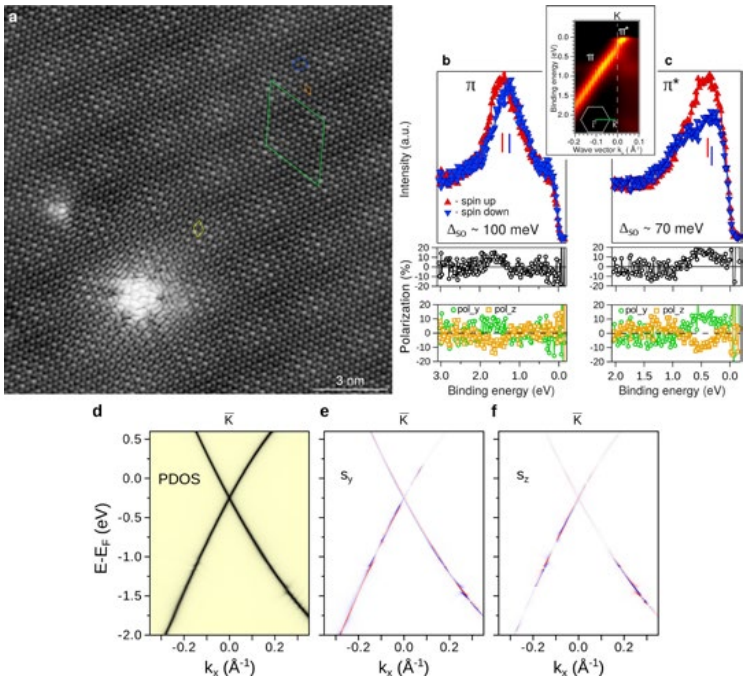


Figure: *(a) Atomically resolved topographic STM image of Pb-intercalated graphene/Ir(111). (b, c) Spin-resolved ARPES spectra of graphene/Pb/Ir(111) acquired for the graphene's π and π* states, respectively. The inset shows the spin-integrated ARPES spectrum. The spin spectra are obtained using the total spin polarization displayed at the middle panels by black circles. The panels at the bottom show the spin polarization components along the y (green) and z (yellow) spin quantization axes. (d) Spin-averaged k,E-resolved density of states maps projected onto C atoms of the graphene/Pb/Ir(111) semi-infinite surface system after unfolding from the (10×10) supercell to the graphene (1×1) unit cell. Panels (e) and (f) show the corresponding in-plane and out-of-plane spin density maps.*

HIGHLIGHT 2

Effect of structural fluctuations on charge injection times in a model dye-sensitized solar cell

Muller M, Sanchez-Portal D, Lin H, Brivio GP, Selloni A, and Fratesi G.

Journal of Physical Chemistry C 122, 7575-7585 (2018)

Electron-transfer dynamics is a key ingredient in many technologically important processes like solar energy harvesting and photocatalysis. In the present work, the authors studied interfacial charge-injection by means of first-principles electronic structure calculations for the case of isonicotinic acid on rutile TiO2(110), a simple model for dye-sensitized solar cells (DSSCs), demonstrating that the inclusion of temperature-induced structural fluctuations is instrumental to obtain good agreement with experimental data.

To date, very few experimental techniques are able to resolve the ultrafast time-scales at which charge injection in DSSCs processes occur. One of the few examples is the so-called core-hole-clock spectroscopy, a chemically selective X-ray technique with the required time-resolution. In spite of this, most of the current theoretical accounts for charge injection ignore the presence of a core-hole in the system. For this reason, the researchers decided to explicitly include the core-excitation in their calculations, thus enabling a direct comparison with core-hole-clock data. Furthermore, they account for a semi-infinite substrate using Green's functions techniques based on density functional theory calculations, providing an accuracy in the description of the resonance's broadening and the electronic structure of the substrate superior to finite-slab calculations.

The effect of temperature is included by sampling structures from Car-Parinello molecular dynamics and calculating instantaneous snapshots of the electronic structure. The energy positions of the molecular resonances, and their couplings to the substrate, fluctuate together with the geometry. Averaging along the trajectory notoriously improves the agreement with experimental data: core-hole-clock experiments estimate the lifetime of the LUMO+2 resonance to be below 5 fs, while the computed time for the equilibrium configuration is ~45 fs. However, the inclusion of structural fluctuations at 300 K brings this value to 6 fs, in good agreement with the experimental data. This highlights the need to perform core-hole-clock experiments as a function of the surface temperature.

Finite temperature also adds an additional inhomogeneous broadening to the cumulative spectra that now resembles a Voigt-like profile modulated by the density of states of the substrate. The inclusion of the core-excitation not only strongly downshifts the resonance energies, but also decreases the inhomogeneous broadening due to an effective reduction of the electron-vibrational coupling.

In summary, a detailed study of charge injection in a model DSSC including finite temperature effects (and core-excitations when present) that allows the satisfactory comparison of the computed results with core-hole-clock experiments is presented in this work. Thus, this study provides new insights and a base to improve the current understanding of electron-injection processes at interfaces.

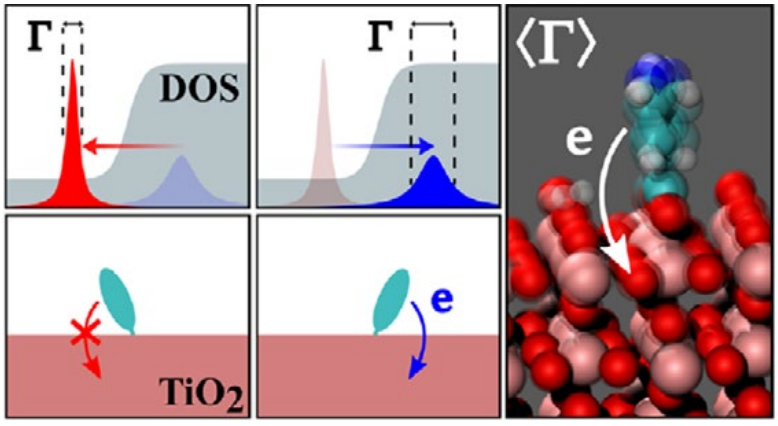


Figure: *Schematic representation of the effect of temperature for charge-injection processes: as the structure fluctuates the molecular resonances move in energy, exploring regions of very different density of states (DOS) in the substrate. Lying on high DOS regions favors charge transfer to the substrate and decreases the resonance lifetime, while sitting in low DOS regions increases it. Thus, it is necessary to take a thermal average of representative structures in order to compare to experimental data.*

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

Cooperative action for molecular debromination reaction on Cu(110)

Sarasola A, Barragan A, and Vitali L.

Journal of the American Chemical Society 140, 15631 (2018)

The metal-catalyzed coupling of halobenzene derivatives leading to biaryls and larger carbon-based structures is a fundamental reaction in chemical synthesis. Here, the mechanistic steps of this reaction, named by Ullmann, have been investigated by means of scanning probe techniques and first-principle calculations. This work shows that the scission of the strongly bound bromine atoms requires the cooperative action of neighboring molecular precursors, in the studied system.

The metal-catalyzed coupling of halobenzene derivatives leading to biaryls and larger carbon-based structures is undergoing a considerable revival in the last decade. The attention to the Ullmann cross-coupling reaction is justified by the reliable synthesis of extended polymers as polyphenyls, graphene structures of well-defined shape, or covalently assembled structures. The unprecedented opportunity to access the molecular functionality with increased mechanical stability and engineered electronic properties offered by this reaction is an essential advance in the realization of organic-based electronics.

The paradigmatic catalyzer of the classical Ullmann reaction is copper. Whereas there is general agreement that at a certain point of the reaction copper-coordinated molecular intermediates and copper halides, as side reaction products, form preceding the cross-coupling reaction, the mechanism responsible for the initial debromination step is still under debate. Indeed, latest investigations on copper surfaces have allowed visualizing the final reaction products as the intermediate Cu-coordinated phase and the aryl-aryl coupling-reaction. Still, the debromination mechanism, which is the rate-limiting step of the reaction, has been scarcely investigated and the question whether the formation of radicals, organocopper complexes or the oxidative addition process precedes the formation of the biaryl remains open.

Researchers of CFM, in collaboration with the University of the Basque Country and Donostia International Physics Center, have demonstrated in this work that the interaction of a halogenated molecular precursor with a metal surface held at an opportune temperature may be an insufficient condition for its debromination reaction. The cooperative interaction with another molecule might be necessary for the dehalogenation process, which is preliminary to their cross-coupling reaction.

Specifically, the mechanistic steps of a molecular debromination have been visualized in the electron density of states by characterizing a prototypical molecule, namely 4,7-dibromobenzo[c]-1,2,5-thiadiazole (2Br-BTD), deposited on a Cu(110) surface. Based on a step-by-step characterization of the adsorption of isolated single molecules, it is shown that the detachment of the halogen atom is subsequential to the formation of –C-Cu-Br complexes and the concerted action of neighboring complexes. Thus, some light has been shed on the debated role of the Cu atom in the debromination reaction.

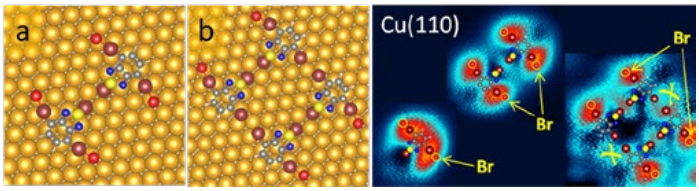


Figure: *Concerted interaction of neighboring intermediate Br-Cu-DBT preceding the molecular debromination. a) Structural model of 2Br-2Cu-DBT dimer. b) The interaction of two self-assembled dimeric pairs promotes the detachment of the Br atoms (red circles between dimers). c) Constant energy maps demonstrating the absence of the electronic state associated to the Br in the inter-dimeric region.*

Electronic Properties at the Nanoscale

The research line “Electronic Properties at the Nanoscale” mainly 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, topology, as well as the dimensionality of nanosized materials are studied as a means to change their properties.

Five theoretical research groups develop the activities of this 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. Recently, a sixth group led by Jorge Sánchez Dolado joined this research line, developing experimental characterization and design of cement based materials. The list of activities developed by the different groups with their corresponding highlights of this year follows:

Group Leader: Andrés Ayuela Fernández, Scientific Researcher, CSIC

06

Electronic Excitations in Surfaces and Nanostructures

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.

In recent years, electronic and magnetic properties of materials have been investigated by this group using first principles methodologies. 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

Controlling the layer localization of gapless states in bilayer graphene with a gate voltage

Jaskolski W, Pelc M, Bryant GW, Chico L, and Ayuela A.

2D Materials 5, 025006 (2018)

The authors show that the localization of topological states that appear near stacking changes in bilayer graphene can be controlled between layers using the value of gate voltage. Our findings introduce the concept of layertronics in the field.

A stacking domain wall in bilayer graphene is a boundary separating two regions with opposite stackings, i.e., AB and BA. When gated, it reveals topologically protected states that occur to be very robust conducting channels along the domain. In previous research, this group found firstly that the number of topologically protected states in corrugated and defectless domain walls is constant and equal to two. They also showed that atomic-scale defects in the domain wall may strongly affect the gapless states. Their number in the gap, which reflects that the number of open conductance channels, can also change with the gate voltage polarization. The origin and exact localization of such states, however, require a more detailed study.

In this work, the group investigated these gapless states for defectless domain walls, using atomistic lattice models, which permit to study their origin by following the formation of carbon bonds between layers. More importantly, they analyze the layer localization and show that it depends on the ratio of the gate potential to the interlayer hopping. Two different regimes were thus defined for small and large gate voltages that may open a route for the use of topologically protected states in practical devices. The control of the carriers' localization in distinct layers along domain walls opens the possibility for the design of *"layertronic"* devices, which could be exploited in addition to other degrees of freedom, like valley, spin and charge, in graphene-based electronics.

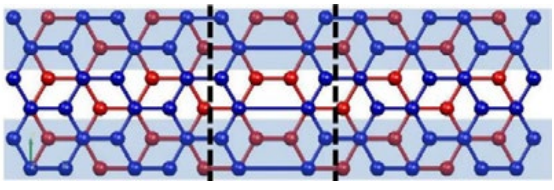


Figure A: *Domain wall separating two stackings of bilayer graphene.*

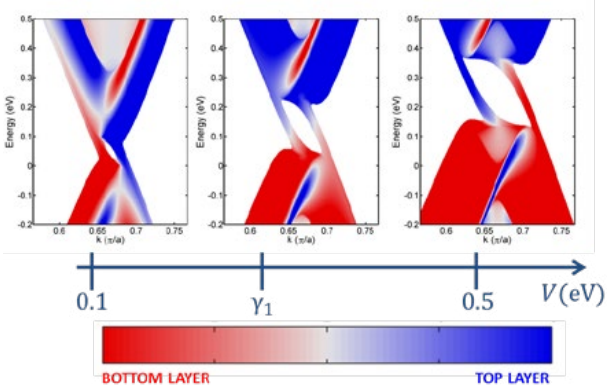
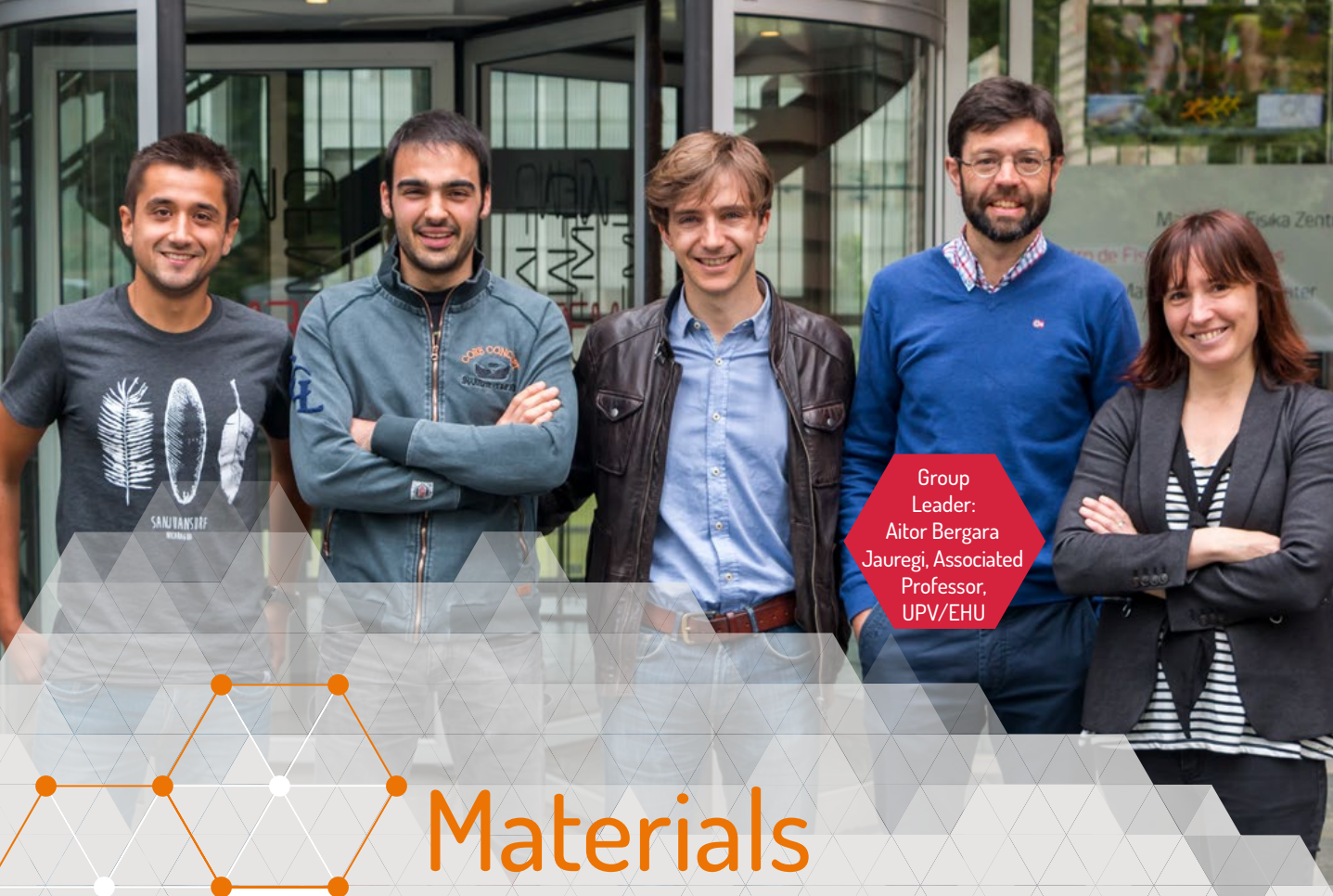


Figure B: *Layer-resolved local density of states as a function of the magnitude of the gate voltage. Note that the two topologically protected states in the gap exchange layer localization with the gate voltage value.*



Group Leader: Aitor Bergara Jauregi, Associated Professor, UPV/EHU

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 analyze 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.

In 2018, Ion Errea, a researcher from the University of the Basque Country (UPV/EHU) joined this group at CFM and took responsibility to command it together in Donostia / San Sebastián, together with Aitor Bergara in Leioa.

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) characterize collective excitations, and (iii) study optical lattices.

HIGHLIGHT

Theoretical calculations shine light on the optical properties of metallic hydrogen

Borinaga M, Ibanez-Azpiroz J, Bergara A, and Errea I.

Physical Review Letters 120, 057402 (2018)

The recent claim by Dias and Silvera of having produced metallic hydrogen at an extremely high pressure of 495 GPa has been a source of intense debate in the scientific community, with pressure determination and the optical approach for characterizing the sample being the main issues put under question. In this work, the authors suggest optical measurements could be a good alternative for characterizing this material in view of the limitations imposed on conventional techniques as neutron or X-ray scattering.

Borinaga et al. in the "Materials Computation and Theory" group performed optical spectra simulations for metallic hydrogen adopting both atomic and molecular structures. The authors have combined time-dependent density functional and Migdal-Eliashberg theories to incorporate electronic band structure and electron-phonon scattering effects in the optical spectra. As shown in figure B, the atomic hydrogen model structure I41/amd shows a sharp decrease of reflectivity for photon energies around 6 eV due to a clear interband plasmon, while for lower energies reflectivity remains high as expected for a metal. On the other hand, the molecular Cmca-4 candidate structure shows a broad region of light absorption at 1-6 eV as the available interband transitions remarkably exceed the ones in the atomic case, and therefore deviates from the typical reflectance spectrum of a metal even if it is also a metal. Therefore, the simulations show molecular and atomic hydrogen display very different features in their visible light and ultraviolet reflectance, suggesting that different phases of hydrogen could potentially be distinguished from their optical spectra.

In the infrared and low frequency visible region, where the very strong electron-phonon scattering governs the optical properties, the experiments are better repro-

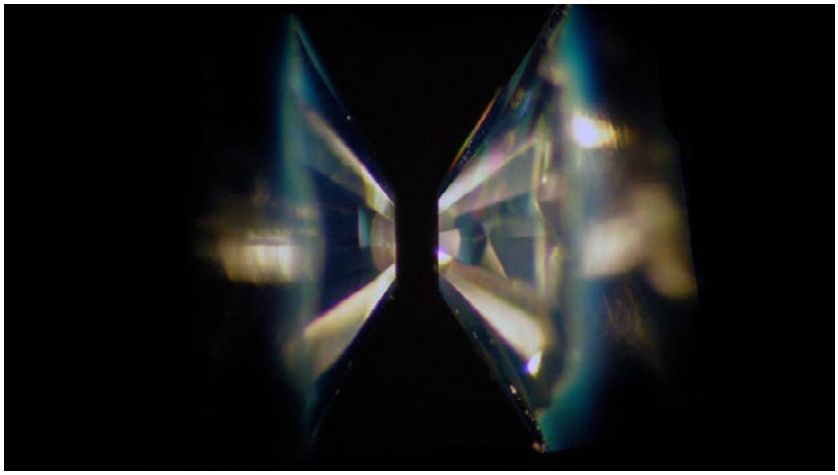
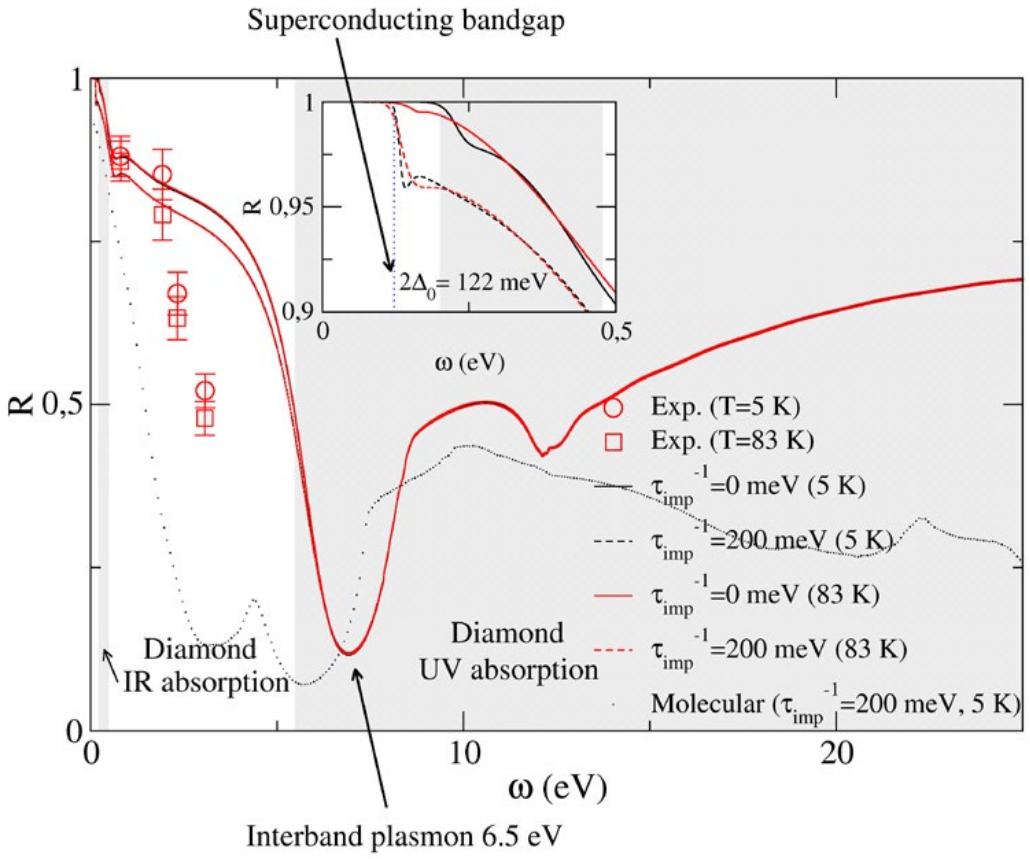


Figure A: *Using two diamonds, scientists squeezed hydrogen to pressures above those in Earth's core. Photo by Sang-Heon Shim, Arizona State University.*

duced with the atomic phase. Moreover, according to their calculations, both atomic hydrogen, which is expected to be superconducting even at room temperature, and molecular hydrogen, which is also expected to be a superconductor but at lower temperatures, show a sharp decrease of reflectivity in the infrared region associated to their extraordinary superconducting properties. More precisely, the larger superconducting energy gap of the atomic phase, and the consequent higher critical temperature, manifests in the optical spectra as this sharp decrease of reflectivity appearing at larger energies; in fact, one expects this feature to appear exactly at an energy of twice the gap value (61 meV and 48 meV in the atomic and molecular cases, respectively).

All this deeply encourages further experimental research in order to extend the optical measurements to a wider region of the electromagnetic spectra. Confirming the predicted features would be not only of tremendous interest by itself, but also a big step towards characterizing this fascinating material.

Figure B: *Calculated reflectivity of atomic I41/amd hydrogen at 500 GPa for different impurity scattering rates and temperatures. A simulation on molecular Cmca-4 is shown for comparison. Experimental values obtained by Dias and Silvera are shown as well. The inset shows a zoom into the infrared region.*



Group Leader: Sebastián Bergeret Sbarbaro, Scientific Researcher, 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.

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

A highly efficient low temperature spin-valve: Towards cryogenic non-volatile random access memory

Sinioni G, Strambini E, Moodera JS, Bergeret FS, and Giazotto F.

Nano Letters 18, 6369 (2018)

A superconductor with a spin–split excitation spectrum behaves as an ideal ferromagnetic spin-injector in a tunneling junction. The combination of two such spin–split superconductors with independently tunable magnetizations may be used as an ideal absolute spin-valve. In this work in collaboration with the Italian CNR and the MIT, Sinioni et al. report on the first switchable superconducting spin-valve based on two EuS/Al bilayers. The relative resistance change between the parallel and antiparallel configuration of the EuS layers up to 900% that demonstrates a highly spin-polarized current through the junction. This device may be pivotal for realization of a logical element for a memory cell in cryogenic, superconductor-based, computers.

Computing-power and data-storage is approaching the physical limits for scaling of semiconducting devices because of large power dissipation and current leakage. Boosted by quantum computing research, cryogenic processors, with computational speed up to 700 GHz, based on superconducting logic elements have been demonstrated and may lead to a considerable power gain that will pay off the power required to cooling down the devices. Recently, ambitious research programs have been launched by large companies triggered by this attractive perspective. One of the bottlenecks in such developments are RAM memories able to work at low temperatures.

In this work the collaborative team presents a spin-valve based on two EuS/Al bilayers coupled by a tunneling interface. It is demonstrated that the switching between a parallel (P) and an antiparallel (AP) configuration of the magnetizations of the EuS layers results in two states with different conductances that may encode the logical-0 and logical-1. The explanation for such spin-valve is based on the theoretical research developed in the Mesoscopic Physics group at CFM.

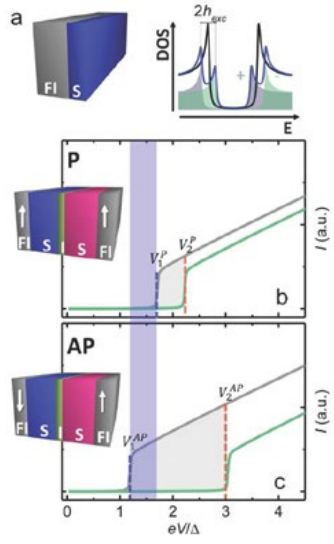


Figure A: *(a) Working principle of the absolute spin valve. A ferromagnetic insulator (Fl, gray block) in contact with a superconductor (S, blue block) induces through exchange interaction an energy splitting in the density of states (DOS, black curve). This results in double-peaked DOS (blue curve). (b)-(c) (b) Tunneling currents I+ (gray) and I− (green) as a function of the voltage bias calculated for the two spin species independently in P and AP configurations.*

EuS is a ferromagnetic insulator with large localized magnetic moments. When a superconductor, like Al, is placed adjacent to it, conduction electrons of the Al interact via exchange with the Eu large moments and are polarized. This process changes drastically the spectrum of the superconductor that shows a spin-splitting of the coherent BCS peaks at the edge of the gap. In such a situation, the superconductor behaves as ferromagnet with a large polarization around the Fermi-level. By switching between the P and AP configuration, one obtains very large values of the TMR ratio. Indeed, the experiment shows TMR ratios up to 900% (see figure B).

This suggests the possibility to use this device as a switching element of a cryogenic memory cell. The readout of such a "bit-line" can be performed, for example, at constant voltage- bias by measuring the tunnel current, which is expected to be zero in the P state and nonzero otherwise. The superconducting bit can be written in response to a magnetic field generated by a control current flowing in a properly designed superconducting "word-write line" that controls the magnetization of the FI with the lower coercive field.

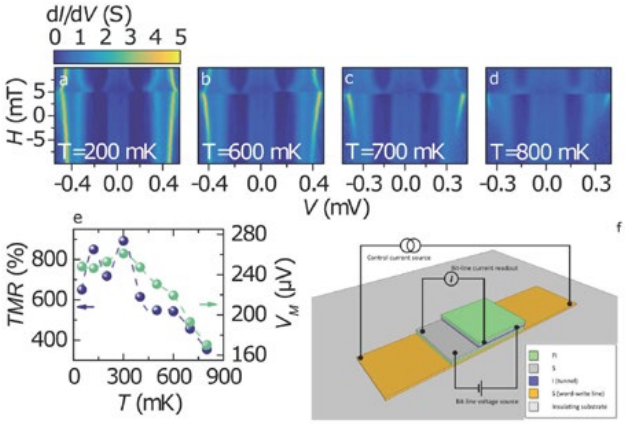


Figure B: *(a–d) Tunneling differential conductance of the spin valve at several temperatures. (e) Maximum TMR(T) as a function of temperature, (f) Scheme of a possible implementation of cryogenic memory cell based on the ASV.*

SELECTED REVIEW

Colloquium: Nonequilibrium effects in superconductors with a spin-splitting field

Bergeret FS, Silaev M, Virtanen P, and Heikkilä TT.

Reviews of Modern Physics 90, 041001 (2018)

In this work in collaboration with Jyvaskyla University group, the members of the group provide a summary of achievements in the field of non-equilibrium transport in spin-split superconductors. Recent experiments and theories by these groups demonstrate a rich variety of transport phenomena occurring in devices based on such materials that suggest direct applications in thermoelectricity, low-dissipative spintronics, radiation detection, and sensing. In this review the theoretical framework is presented, based on quantum kinetic equations, which provides an accurate description of the distribution of charge, spin, and energy, which are the relevant nonequilibrium modes, in different hybrid structures. Experiments on spin-split superconductors are also reviewed.

One of the main research activities of the Mesoscopic Physics Group in recent years has been the study of properties of devices consisting of ferromagnetic insulator/superconductor (FI/S) bilayers. This interest originates from the fact that such systems can be seen as superconducting magnets, with large spin polarizations at the Fermi-surface. Transport properties of FI/S devices is extremely rich and the Mesoscopic Physics group, in collaboration with other groups, has suggested several applications in thermoelectricity, low-dissipative spintronics, radiation detection, and sensing, along the past five years. These works have motivated the experimental activity in this field, and opened up diverse collaborations.

In this review, the authors have outlined the main issues in the field, by putting the focus on non-equilibrium properties. Often the nonequilibrium effects can survive to large distances, as their decay scales are determined via the various inelastic and spin-flip scattering lengths. Nonequilibrium properties are related to the deviation of the electron distribution function from its equilibrium form, which leads to a nonequilibrium distribution (imbalance) of charge, energy, or spin degrees of freedom: the nonequilibrium modes. The review explores the coupling between these modes in superconductors with a spin-splitting field and discusses unusually strong thermoelectric response and long range spin signals.

As extremely interesting examples, the review focuses on tunnel contacts with spin-split superconductors. These systems exhibit a strong spin-dependent electron-hole asymmetry. This asymmetry leads to a large spin Seebeck effect: a temperature difference across a tunneling interface between a normal metal and a spin-split superconductor drives a pure spin current between the electrodes, without transport of charge. In certain situations the relevant observables are not spin averaged, resulting in an effective electron-hole asymmetry showing up also in the charge current. The spin components are weighted differently in a setup consisting of the spin-filter junction connected to the spin-split, and as a result of this effective electron-hole symmetry breaking, the system exhibits a very large thermoelectric effect.

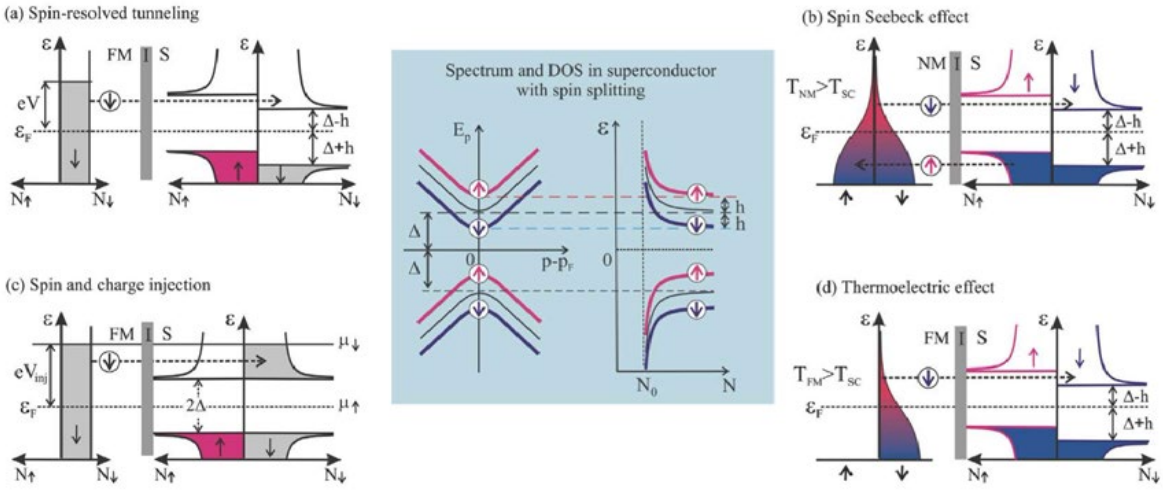


Figure: *Central panel: Quasiparticle spectrum and density of states in a superconductor with spin splitting. (a)–(d) Schematic of various nonequilibrium phenomena occurring at normal metal/insulator/superconductor and ferromagnetic metal/insulator/superconductor interfaces discussed in the review.*

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 have been also developed, assessing exchange correlation (XC) functionals for TDDFT calculations. Improvements on transport theory within the real-time TDDFT formalism have also been 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

Ultrasensitive H_2S gas sensors based on p-type WS_2 hybrid materials

Asres GA, Baldoví JJ, Dombovari A, Järvinen T, Lorite GS, Mohl M, Shchukarev A, Pérez Paz A, Xian L, Spetz AL, Jantunen H, Rubio A, and Kordás K.

Nano Research 11, 4215 (2018)

Air pollution has a dramatic impact on human health and disease. Around seven million deaths a year all over the world are linked to exposure to both gas-phase species and particulate matter. Therefore, the development of novel sensors for gas detection and monitoring will bring a major benefit to sectors such as environmental protection, health and food industries, as well as everyday life for millions of people. In this context, nanostructured metal sulfide semiconductors offer a very promising platform for resistive chemical sensor applications due to their higher intrinsic electrical conductivity and chemical stability with respect to their oxide counterparts, which stand out as the most common active sensing materials nowadays.

In this work, Asres et al. explore the gas sensing behavior of a transition metal disulfide (WS_2) nanowire-nanoflake hybrid material by using a simple two-terminal Taguchi-type sensor arrangement. This work by the group demonstrates the excellent sensitivity as well as high selectivity of the material towards H_2S relative to CO, NH_3, H_2, and NO. The gas response measurements are complemented with X-ray photoelectron spectroscopy analysis and first-principles calculations based on density functional theory. This combination of experimental and theoretical techniques allows for identifying a partial –and reversible– substitution of S by O at the anionic sites of the lattice, which plays a major role to explain the high sensitivity and selectivity of the WS_2 nanowire-nanoflake heterostructures towards H_2S.

These results open up new avenues for the use of transition metal disulfide nanomaterials as effective alternatives to metal oxides in future applications for industrial process control, security, and health and environmental safety.

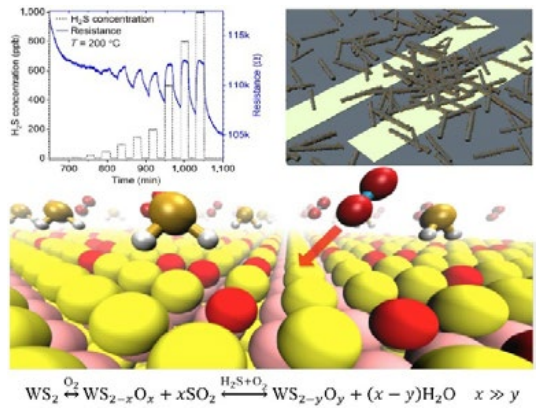


Figure: *(Upper panel) left: H_2S sensing performance at parts per billion levels at 200 C and right: Microstructure of WS_2 nanowire/nanoflake hybrids. (Lower panel) Schematic illustration of H_2S sensing mechanism on the surface of WS2 in the presence of O_2. The WS2 lattice is doped with O in the presence of air (O_2), partially substituting S in the anionic sites.*

10

Souza Research Group

The activity of this 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 localized 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

Unusual optical effects in conducting helical crystals

Tsirkin SS, Puente PA, and Souza I.

Physical Review B 97, 035158 (2018)

An object is said to be chiral if, like our two hands, it not superposable on its mirror image. Chiral objects therefore possess a definite "handedness": the mirror image of a right-handed chiral object is a left-handed chiral object, and vice-versa. Certain crystal structures are chiral, occurring in both right- and left-handed varieties. A simple example is the structure adopted by the elemental semiconductors selenium and tellurium, where the atoms form helical chains disposed on a hexagonal net. The chains possesses a definite handedness, rendering the crystal structure chiral.

Helical crystals exhibit fascinating phenomena, such as optical rotation: when linearly-polarized light propagates through the crystal along the helical axis, the plane of polarization rotates by a certain amount per unit length traveled, that amount being equal and opposite for right- and left-handed samples.

In this work, the group theoretically studied several phenomena that occur in conducting helical crystals, using p-doped tellurium as a specific example. In such crystals, the atomic chains behave as "microscopic solenoids": the passage of an electrical current along the helical axis induces a parallel magnetization, as illustrated in the figure below. Although the induced magnetization is rather small, it can be detected by optical means (Faraday rotation of transmitted light) due to the high transparency of the sample. In agreement with the experiment, the theoretical study found that (i) when infrared light propagates antiparallel to the current at low doping, the current-induced Faraday rotation enhances the natural optical rotation, and (ii) the plane of polarization rotates in the opposite sense to the bonded atoms in the spiral chains.

Another phenomenon exhibited by helical crystals is the circular photogalvanic effect: the generation of a photocurrent that reverses sign with the helicity of light propagating along the helical crystal axis. The present work was able to explain the experimental finding that the circular photocurrent in p-doped tellurium reverses sign with increasing temperature. This sign change was attributed to the presence of chiral band crossings ("Weyl points") near the bottom of the conduction band acting as sources and sinks of Berry curvature.

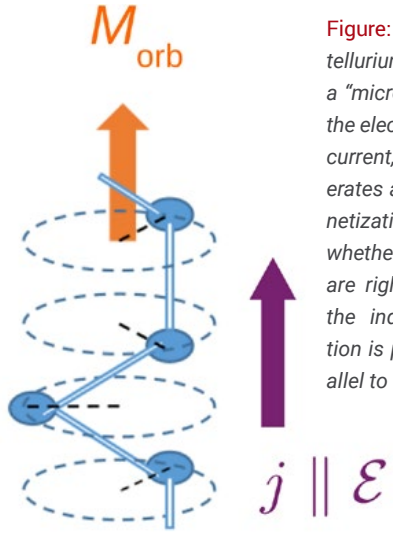


Figure: *A helical chain of tellurium atoms acting as a "microscopic solenoid": the electric field induces a current, which in turn generates a bulk orbital magnetization. Depending on whether the helical chains are right- or left-handed, the induced magnetization is parallel or antiparallel to the current.*

Group Leader: Jorge Sánchez Dolado, Tenured Scientist, CSIC

11

Ceramic and Cement-Based Materials

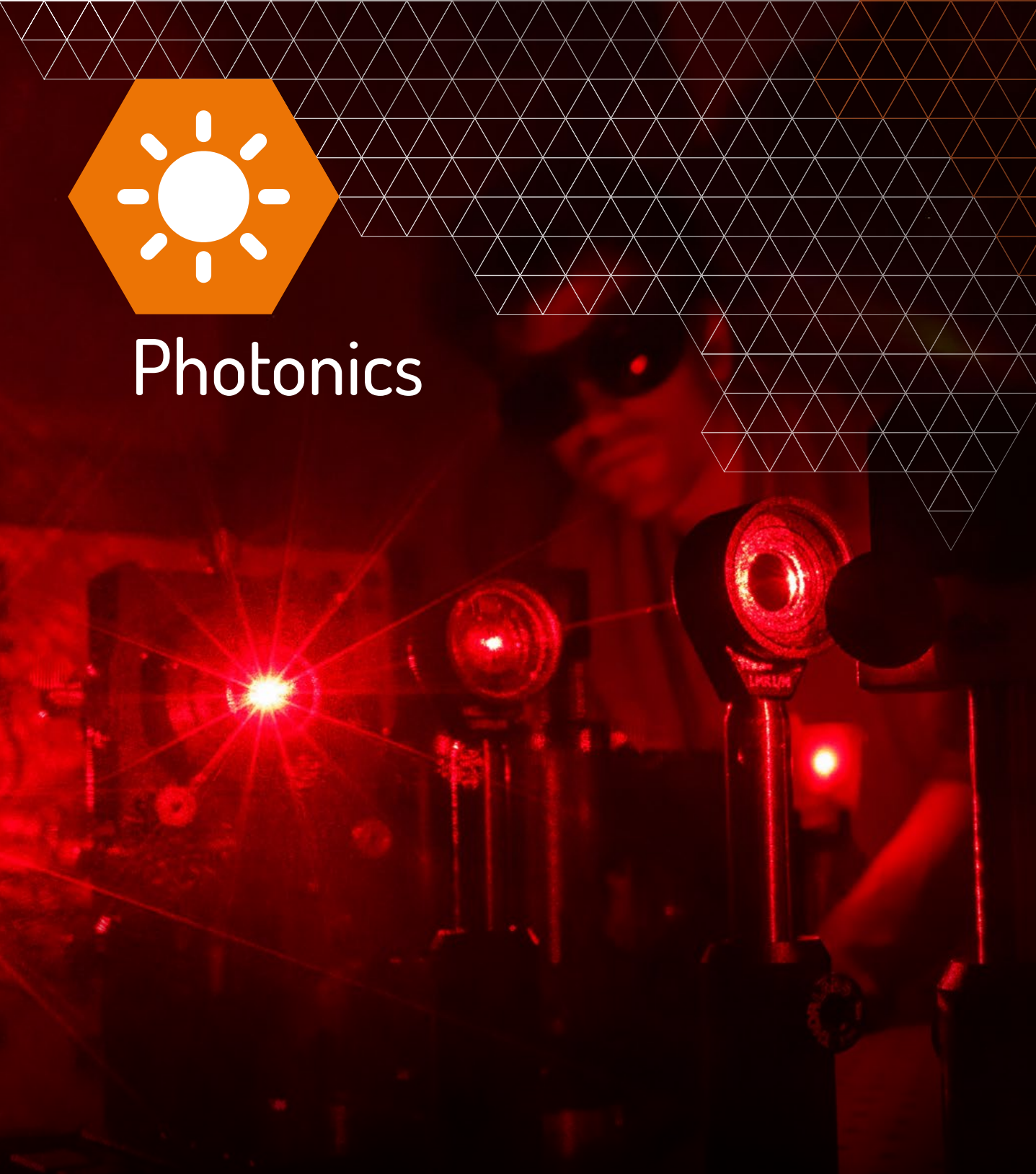
This new group at CFM has been created during 2018 aiming at experimentally and theoretically researching a variety of properties of cement-based and ceramic materials. Combining knowledge from different disciplines like solid-state physics, soft-matter physics, geochemistry and chemical engineering, the "Ceramic and Cement-based Materials" group focuses on the computational design and synthesis of new ceramic and cement based materials with lower CO_2 fingerprint. Among the initial objectives of the group, one can name the following:

i. Use of atomistic and colloidal simulations to study the structure and properties of cement-based materials.

ii. Implementation of new hydrothermal and supercritical fluids (SCF) technologies for the ultra-fast synthesis of ceramic nanoparticles.

iii. Development of new sintering methodologies through the use of autoclaves or microwaves that allow notable energy savings and a drastic reduction of CO_2 emissions.

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 nanoscale 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.

Group Leader:
Javier Aizpurua
Iriazabal, Research
Professor, CSIC

12

Theory of Nanophotonics

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 configurations: 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 by this group: (i) understanding and characterization 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) characterization of the dynamics and the coupling of emitters to be used in quantum information technology.

HIGHLIGHT

Vibrational Electron Energy Loss Spectroscopy in Electron Microscopy reveals new aspects of water at the nanoscale level

Jokisaari JR, Hachtel JA, Hu X, Mukherjee A, Wang CH, Konečná A, Lovejoy TC, Dellby N, Aizpurua J, Krivanek OL, Idrobo JC, and Klie RF.

Advanced Materials 30, 1802702 (2018)

A new microscopy technique developed at the University of Illinois at Chicago, in collaboration with researchers at Oak Ridge National Lab. in Tennessee, the Nion Company in Seattle, and the group at CFM, allows researchers to visualize liquids at the nanoscale level - about 10 times more resolution than with traditional transmission electron microscopy - for the first time, and to understand the details of the vibrational properties of the liquid sample in a complex nanoenvironment.

By trapping minute amounts of liquid between two two-dimensional layers of boron nitride, the liquid sample can be imaged at extremely high resolution using a traditional transmission electron microscopy and spectroscopy techniques. This approach could provide information on the vibrational state of individual molecules.

The new technique can be used to follow nanoscale-sized tracers used in biological research, and to visualize processes at liquid-solid interfaces at unprecedented resolution. Using their specialized sample holder, or boron nitride cell, the researchers describe the unique vibrational properties of water and heavy water at the nanoscale level. Researchers of the "Theory of Nanophotonics" group helped to interpret the vibrational information obtained in the energy loss spectra, by a modelization of infrared response of the liquid water sandwiched in the boron nitride layers. This study shows the importance of the nanoscale environment to properly account of the energy and intensity of the vibrational lines obtained with this novel microscopy technique.

By using a scanning transmission electron microscope with one of the world's best energy resolutions at the Department of Energy's Oak Ridge national laboratory in Tennessee, the vibrational spectrum of liquid water at the milli-electron volt's range could be measured. Normally, water in large amounts vibrates at 420 milli-electron volts, but the researchers witnessed that water trapped in the BN cell vibrated at 406 milli-electron volts.

This new electron microscopy technique allows to see physical and chemical processes happening in a liquid environment at the nanoscale level. Far smaller volumes can be measured by other methods, but at such small scales, the behavior of water changes as individual atomic bonds, local electric fields and the proximity of surfaces begin to affect its normal behavior. Some of these effects have been accounted for within the dielectric response theory used by the "Theory of Nanophotonics" group at CFM to reveal the complex interactions of the nanoenvironment, which determines the final details of the vibrational spectra.

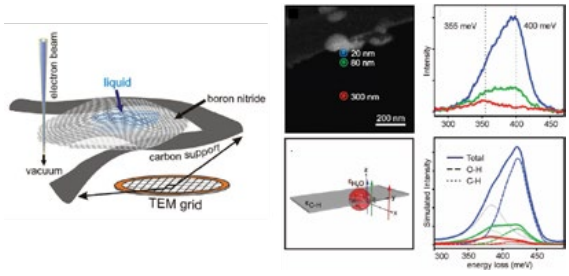


Figure: *Left: Schematics of the sample consisting of liquid water encapsulated in a double layer of boron nitride supported on carbon at the TEM grid of the scanning transmission electron microscope. Right: Top-left: Image of the cell probed by electron beams at three different positions (blue, green, and red). Top-right: Experimental vibrational Electron Energy Loss Spectroscopy (EELS) of the sample to the left for the three different electron beam positions. Bottom-left: Model system used to calculate the dielectric response of a water bubble supported by a carbon layer. Bottom-right: Theoretical vibrational EELS of the model system to the left reproducing the vibrational fingerprints of the liquid nanoscale system, revealing the O-H and C-H stretching modes.*

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

13

Nanomaterials and Spectroscopy

The activity of the "Nanomaterials and Spectroscopy" group focuses on the experimental study of spectroscopy and photonic applications of nanoscale 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 nanoscale 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

Energy transfer between single semiconductor quantum dots and organic dye molecules

Melnikau D, Hendel T, Linkov PA, Samokhvalov PS, Nabiev IR, and Rakovich YP.

Zeitschrift für Physikalische Chemie 232, 1513 (2018)

In this work, steady-state and time resolved optical studies of the emission properties of an ensembles and single semiconductor quantum dots and attached organic dye molecules were conducted. It was revealed that the luminescence intensity of a hybrid structure does not follow the blinking behavior of quantum dots. An efficient single-photon generation from single nanostructures was also demonstrated involving an energy transfer from donor to acceptor as main excitation source.

An understanding of the mechanisms of energy transfer and conversion on the nanoscale is one of the key requirements for an implementation of highly efficient photonic nanodevices based on hybrid organic/inorganic nanomaterials. Quantum dots are particularly promising for photonic applications due to their size dependent spectral tunability, high extinction coefficient, broad absorption tail, relatively narrow emission bands and exceptional photostability. On the other hand, the main advantages of organic materials are their versatility, easy processing, high brightness and small size.

The investigation and utilization of hybrid materials built from these constituents can, in principle, lead to the high-performance devices that would benefit from the superior optical and electrical properties of quantum dots and functional diversity and flexibility of organic compounds. The combination of organic and inorganic components forming nanostructures can help to overcome some limitations of these materials, such as limited stability of organic materials under laser excitation or narrow spectral region where photoluminescence of organic dyes can be efficiently excited. They can also take advantage of the rather long PL lifetime of semiconductor quantum dots which is a highly desirable functionality for some of the biological applications, hindering the development of high-speed communication devices.

In this work, the simplest case of hybrid organic/inorganic nanostructure, which utilizes van-der-Waals interactions between donor and acceptor was investigated. The group demonstrated that, although bounding of an organic dye molecules and quantum dots is supposed to be weak, resonant energy transfer in fabricated hybrid nanostructures is still possible. It was shown that, even in a weak binding regime, efficient single photon generation from single hybrid nanostructures can be achieved, which involves energy transfer of a reasonable efficiency from donor (quantum dots) to acceptor (dye molecules) as a main excitation source. This experimental finding might be helpful for the development of efficient single photon sources and the advancement of other practical applications in the fields of optical communications, quantum optics, and sensing.

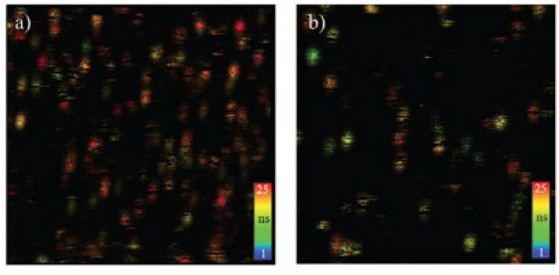


Figure: *Fluorescence lifetime microscopy images (a, b) of a pure QDs (a) and QDs/dye (b) hybrids in a PMMA film.*

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

14

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 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

Sustainable luminescent solar concentrators based on organic–inorganic hybrids modified with chlorophyll

Frias AR, Pecoraro E, Correia SFH, Minas LMG, Bastos AR, Garcia-Revilla S, Balda R, Ribeiro SJL, Andre PS, Carlos LD, and Ferreira RAS.

Journal of Materials Chemistry A 6, 8712 (2018)

Frias et al. report novel chlorophyll-based Luminescent Solar Concentrators (LSCs) with emission properties in the red/NIR spectral region. Chlorophyll molecules extracted from Spirulina maxima are immobilized in organic–inorganic di-and tri-ureasil matrices enabling the production of sustainable LSCs. The LSCs were coupled to a Si-based commercial PV device revealing optical conversion efficiency and power conversion efficiency values of 3.70% and 0.10%, respectively, illustrating the potential of this approach for the development of nature based LSCs meeting the requirements of reliable, sustainable and competitive energy systems.

Luminescent Solar Concentrators (LSCs) are luminescent waveguide layers that convert sunlight into specific wavelengths, which are then guided by total internal reflection to a PV device located at the edges of the LSC. Their ability to concentrate sunlight onto small areas makes LSCs a useful complement to silicon-based PVs in a series of applications, such as urban integration and flexible fabrics towards mobile solar-energy. Challenges for the luminescent layer include the use of low-cost and sustainable nature-based organic molecules. The potential replacement of QDs and synthetic organic dyes with red/NIR luminescent nature-based organic molecules extracted from natural pigments could make LSCs cheaper and sustainable, as well as providing other intrinsic properties such as synthetic versatility, and high absorption coefficients and emission quantum yield.

In this collaborative work carried out by the groups led by Luis Carlos (Aveiro Institute of Materials, University of Aveiro) and Rolindes Balda (CFM), nature-based LSCs made of chlorophyll molecules dispersed in organic–inorganic ureasil hybrids were studied. The chlorophyll molecules were extracted from Spirulina maxima, which is an abundant cyanobacterium and an attractive natural source. The chlorophyll-based active layer displays a large overlap with the solar irradiance on the surface of the Earth, (absorption at 300–450 nm and 600–850 nm) and emission spectra centered around 675 nm. At low chlorophyll concentration values (1017 molecules per cm3), the optical properties (fluorescence lifetime, quantum yield and brightness) are preserved after the incorporation into the hybrids hosts. The optimized hybrid sample with an optical conversion efficiency, opt = 3.70 ± 0.01%, was tested as an LSC coupled to commercial Si-based PV devices, revealing an effective contribution to its performance, namely, an increase in the power conversion efficiency PCE (0.10 ± 0.01%). The use of natural red/NIR emitting dyes, such as chlorophyll molecules, as active layers in LSCs, demonstrates the huge potential of nature-inspired LSCs as a relevant step toward sustainable PV energy conversion. A quantitative evaluation of the chlorophyll-based LSC performance was corroborated by Monte Carlo raytracing simulations, indicating that the optical efficiency can still be maintained for larger devices.

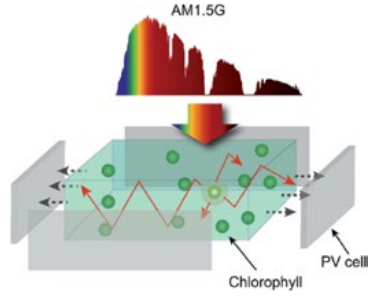


Figure: *Representative scheme of the Chl-based LSCs attached to the c-Si PV cells. The arrows inside the LSC indicate the total internal reflection of the emitted light. The dashed arrows represent the PV cell coupling region.*

Group Leader: Gabriel Molina Terriza, Ikerbasque Professor, MPC

15

Quantum Nanophotonics Laboratory

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, developing research on Quantum Information with entangled Photons.

The group is developing an experimental laboratory to deal with optical scattering experiments at cryogenic temperatures where non-classical states of light interact with nanoscale structures. The completion and development of the laboratory has extended along 2018.

HIGHLIGHT

Threading entangled photons through nanoholes

Buse A, Juan ML, Tischler N, D'Ambrosio V, Sciarrino F, Marrucci L, and Molina-Terriza G.

Physical Review Letters 121, 173901 (2018)

A team of international researchers led by this group developed an effort to understand the properties of the fundamental blocks of light (photons) when they interact with nanometric objects. In particular, it was showed that a very delicate quantum property of photons, their entanglement, can be protected even when they go through a subwavelength aperture. This research can open new paths to quantum communications, quantum sensors and computational schemes.

Quantum entanglement was deemed by Albert Einstein as the "spooky action at a distance" of quantum systems, the feature that makes them completely depart from our common day expectations. The push for quantum technologies has placed quantum entanglement of photons, electrons, atoms and even macroscopic systems at the forefront of a quest to make these technologies market-ready. As such, quantum entanglement is essential for safe quantum communications, efficient quantum computers and to push the limits of quantum sensors to its ultimate frontiers. Unfortunately, entanglement is a very delicate property of quantum systems, which is typically destroyed when they interact with their environment.

An international team led by the head of the Quantum Nanophotonics Laboratory proved that this interesting property can be shielded in the case of photons, even when they interact with tiny particles, smaller than the wavelength of light. Entangled photons are essential in quantum communication protocols or in the production of quantum photonic chips with improved computing and sensing capabilities. Nevertheless, in order to make these systems available one needs to reduce the size of the chips. In that nanophotonics regime, properties such as the spatial shape or polarization of the photons, which are used to carry information, are so distorted and affected by the interaction with tiny particles, that it is extremely difficult to keep their entanglement.

In the article published in Phys. Rev. Lett. by Büse et al, the researchers prepared an entangled state of photons which kept its entanglement when being transmitted by a hole smaller than the wavelength of light. The approach that was used was to encode the quantum information in a way that it was protected by the symmetry of the circular nanohole. The researchers showed that, in principle one can adapt the information encoding to the kind of environmental interaction that the photons must face, even at the nanoscale regime. This could render photonic entanglement useful for nanodevices which could improve our sensing capabilities of biomolecules, or improve the capabilities of quantum light transmission in miniaturized quantum chips.

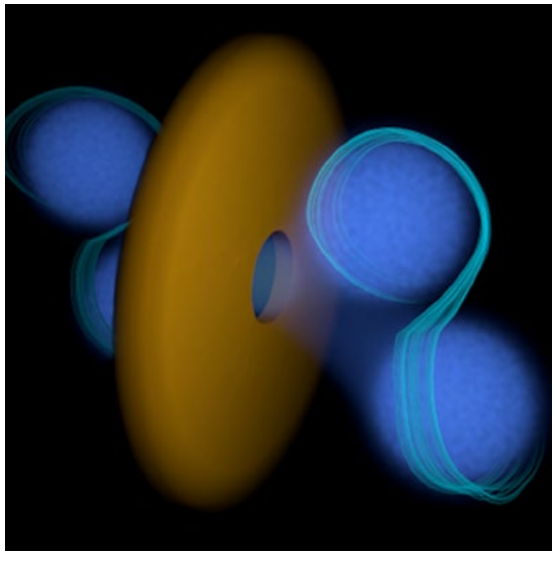


Figure: *Entanglement protection through nanoholes. Image credits: Mathieu Juan.*

Polymers and Soft Matter

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

16 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 characterization 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 center 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 center, 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 characterize particular forms of soft matter, such as rubber.

HIGHLIGHT 1

Crowding the environment of single chain nano-particles: A combined study by SANS and simulations

González-Burgos M, Arbe A, Moreno AJ, Pomposo JA, Radulescu A, and Colmenero J.

Macromolecules 51 (4), 1573-1585 (2018)

Researchers in the group investigate the conformations of Single-Chain Nano-Particles (SCNPs) in crowded macromolecular solutions. Inert linear chains and the SCNPs themselves are used as crowders. A continuous cross-over from unperturbed conformations in dilute conditions toward fractal globular states is found for the SCNPs with increasing concentration. The collapse starts at the monomer concentration corresponding to the overlap concentration of the pure SCNPs, irrespective of the size and topology of the crowders. A potential scenario emerges for the effect of the steric interactions on intrinsically disordered proteins in crowded environments.

Single-Chain Nano-Particles (SCNPs) are polymeric soft nano-objects consisting of unimacromolecular chains collapsed to a certain degree by means of intramolecular bonding. Sensing capabilities, controlled drug delivery, and catalytic applications, among others, of SCNPs have been recently demonstrated. The global conformations exhibited by SCNPs in dilute solution share some structural features with those displayed by Intrinsically Disordered Proteins (IDPs). IDPs are ubiquitous in nature and responsible for functions of utmost relevance in biological systems. Their biological function is founded on their internal dynamics and flexibility, which enable them to respond quickly to environmental changes and to bind with different cellular targets. Though lacking of ordered structure, SCNPs still show weakly deformable domains (analogues of ordered IDP domains) connected by flexible disordered linkers. Dynamically, both SCNPs and IDPs share a high degree of internal friction that strongly hampers chain motions. These similarities can be invoked to consider SCNPs as model systems, free of specific interactions, to mimic properties of IDPs in different environments (crowding, confinement, etc.).

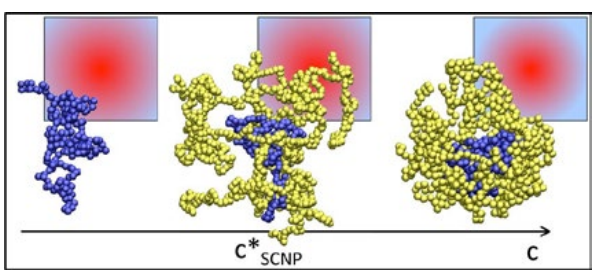


Figure A: *Simulation snapshots for a SCNP (blue beads) in the limit of high dilution (left panel) and in the presence of linear crowders (yellow beads, middle and right panels). Middle panel corresponds to a total monomer concentration C identical to the overlap concentration (C^*_{SCNP}) of the solution of pure SCNPs. The right panel corresponds to a concentrated solution far above C^*_{SCNP}. SANS patterns are schematically reproduced for each case (colors mean from low (blue) to high (red) intensity values).*

With these ideas in mind and the aim of disentangling the role of the steric effects created by the crowders, González-Burgos et al. investigated the conformations of SCNPs in macromolecular solutions. Through a combined study by Small Angle Neutron Scattering (SANS) experiments and MD simulations, the following physical scenario emerged:

i. By using inert linear chains of very different molecular weights as crowders, they find a crossover from almost unperturbed SCNP conformations in dilute conditions toward a continuous collapse of the macromolecule with increasing crowding. The overlap monomer concentration of the SCNP is the key factor determining the crossover toward compaction. The analysis of the form factor reveals that in crowded conditions the SCNPs tend to collapse to conformations similar to the so-called fractal globule, instead of the well-known Gaussian conformations adopted by linear chains.

ii. If SCNPs are used as crowders, the experimental system shows unavoidable aggregation due to cross-linking of unreacted functionalized monomers. However, the simulated system, free of this ingredient, demonstrates that the features observed when crowders are linear also persist in this case. The generalizability of these findings is supported by the generic character of the "bead-spring" coarse-grained model used in the simulations, and suggests a potential scenario for the effect of the steric interactions on IDPs in crowded environments.

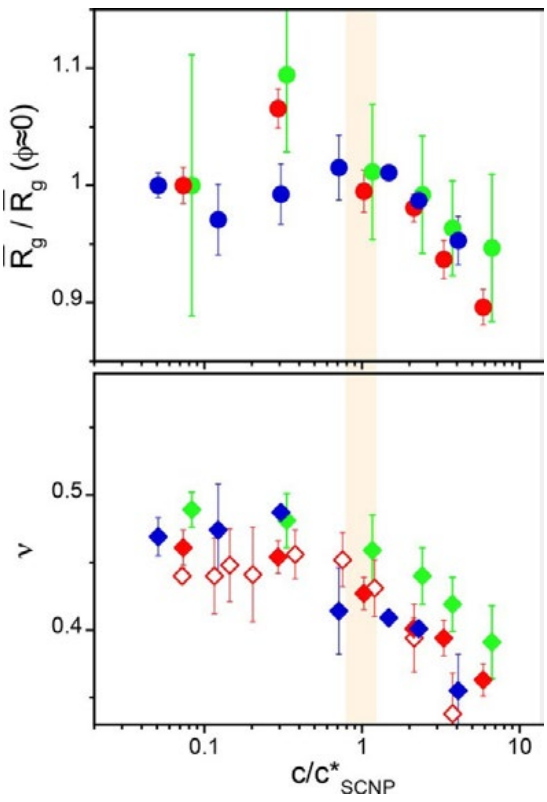


Figure B: *Normalized radius of gyration of the SCNPs (top) in solutions crowded with linear chains, and the corresponding scaling exponents (bottom), both quantities being obtained by analyzing the SANS form factors. Different data sets correspond to different size ratios of the SCNPs and linear crowders. The data are represented vs the normalized concentration C/C^*_{SCNP} to highlight the beginning of the collapse in all cases at the overlap concentration of the solution of pure SCNPs.*

HIGHLIGHT 2

Thermodynamic ultrastability of a polymer glass confined at the micrometer length scale

Monnier X, and Cangialosi D.

Physical Review Letters 121, 137801 (2018)

Monnier et al. employ fast scanning calorimetry to assess the thermodynamic state and the molecular mobility of glassy micrometric poly(4-tert-butylstyrene). The authors show that, for such a large confinement length scale, glasses with extremely low energy are attained. This allows bypassing the geological timescales required for bulk glasses. More importantly, the access to such low states takes place while the molecular mobility remains bulk-like, indicating marked decoupling between vitrification kinetics and molecular mobility.

Cooling a liquid below its melting temperature, provided that crystallization is avoided, results in its transformation into a non-equilibrium glass; a phenomenon known as the glass transition or vitrification. Such event implies that the energy decrease of the supercooled liquids with decreasing temperature – and thereby the access to low energy states – is hindered. In bulk glass-formers, accessing such state requires experimentally unfeasible time scales already at temperatures close to the glass transition temperature (Tg). Conventional wisdom relates the glass transition exclusively to the glass molecular mobility. However, apart from the conceptual difference between vitrification and molecular mobility, recent experimental activity has shown that these two aspects are decoupled when confining polymers at the nanoscale. In particular, these systems revealed depressed glass transition temperature (Tg) with respect to the bulk polymer, while the molecular mobility remains bulk-like.

In this contribution, researchers in the group investigate vitrification kinetics over a wide range of cooling rates and molecular mobility of an amorphous polymer, that is, poly-tert(butyl styrene) (PTBS), with size in the micrometers range, by fast scanning calorimetry.

Monnier et al. characterize vitrification kinetics in terms of the fictive temperature (T_f), which defines the thermodynamic state attained by a glass obtained at a given cooling rate. The authors show that the T_f of these systems vastly deviates from that of the bulk. In the Figure T_f is presented as a function of the cooling rate. At the lowest investigated cooling rate, the smallest investigated sample (2.5 μm typical size) exhibit a T_f depression as large as ~80 K, as exemplified in the Figure. More importantly, beside such depression in T_f, no alterations of the molecular mobility are detected (see Figure-left panel).

Our results, apart from showing the decoupling between vitrification kinetics and molecular mobility for a large size sample, indicate that accessing thermodynamic states with low T_f is strongly facilitated by the presence of a large amount of free interface. The main consequence is that this kind of glass offers a formidable means to resolving challenges of the glass transition, thereby circumventing the geological timescales required to access low energies in bulk glasses.

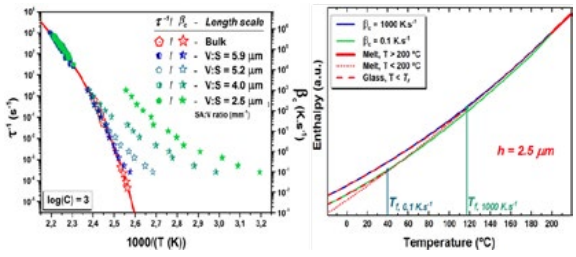


Figure: *(left panel) and (right panel) enthalpy plot showing the thermodynamic state achieved PTBS with size 2.5 μm at large (1000 Ks-1) and low (0.1 Ks-1) cooling rates.*

Resolving component dynamics of a simplified industrial polymer system by combining neutron scattering and dielectric spectroscopy

Gambino T, Alegria A, Arbe A, Colmenero J, Malicki N, Dronet S, Schnell B, Lohstroh W, and Nemkovski K.

Macromolecules 51, 6692 (2018)

By combining quasielastic neutron scattering on isotopically labeled samples and dielectric spectroscopy techniques, Gambino et al. have been able to disentangle the component dynamics of a polymer blend of interest for the tire industry, and shown that the concepts developed for canonical mixtures are transferable to such materials.

The optimization of the performance of rubbers in tires requires reducing the rolling resistance and increasing the dissipation of energy during braking. Blending polymers is an efficient and cheap way to obtain materials with new properties, but the rational design of interesting mixtures for tire industry involves the understanding of the dynamics of both components at distinct frequency ranges (10-102 Hz for the rolling resistance and 104-107 Hz for the adherence).

In the framework of collaboration of the Polymers and Soft Matter group with MICHELIN, the authors have applied the concepts and methodologies 'academically' developed for the investigation of polymer blend dynamics to disentangle the component dynamics in a simplified industrial system consisting of a 50/50 mixture of a random copolymer, SBR, with an oligomer, PS. The main conceptual ingredients are dynamic heterogeneity (the two components retain their 'identity') and concentration fluctuations (leading to a variety of environments in the sample). The methodology involves the combination of different experimental techniques including DSC, Dielectric Spectroscopy (DS) and Quasi-Elastic Neutron Scattering (QENS). As an essential part of this methodology, QENS on isotopically labelled samples was a requirement in order to isolate the response of one of the components in the mixture, (see Figure A for the case where the SBR component is isolated).

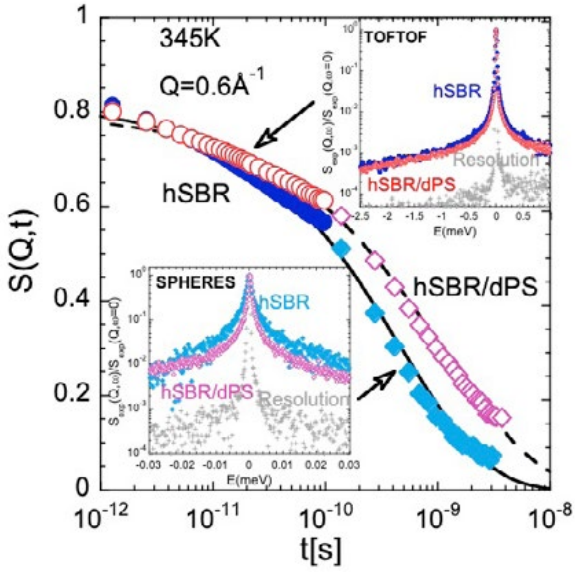


Figure A: *Intermediate scattering functions of pure SBR and the SBR component in the blend with deuterated PS. Lines are fits of stretched exponentials to the experimental results for t ≥ 2 ps. Insets show the normalized measured functions in the frequency domain, obeying the same symbol code.*

Thanks to the synergetic combination of QENS with DS data (where the isotopic labeling does not play a role) covering a broad frequency range, a complete description of the segmental dynamics of the two polymer components in such a complex mixture was possible in the full range of frequencies of industrial interest (see figure B). In this way, Gambino et al. resolved the fragility of the two components in the blend and identified the distribution of effective glass-transition temperatures of each blend component that nicely match the whole glass-transition range of the mixture as determined by DSC. This work thus demonstrates that the concepts established for blend dynamics in systems composed by 'canonical' polymers can be transferred to other more complex mixtures of industrial interest.

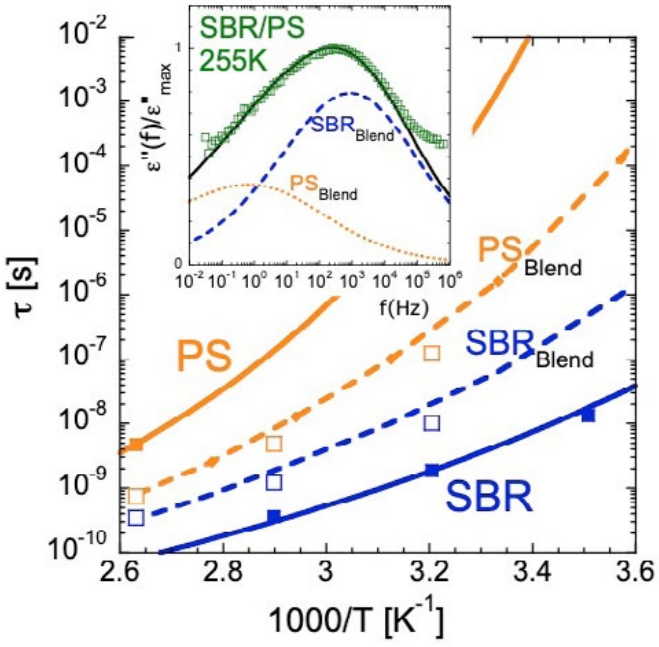


Figure B: *Relaxation map (lines: descriptions of the DS times; symbols: QENS characteristic times at the Q-value matching the latter) of the blend components (dashed lines and empty symbols) compared with the neat materials (solid lines and full symbols). The inset shows DS results at 255K decomposed in the two contributions.*

FACILITIES & EXTERNAL SERVICES

CFM infrastructure has been envisioned to characterize nanoscale materials with high sensitivity. Thus, CFM headquarters were 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 specialized experimental techniques, ready to give response to the needs in advanced materials characterization. These needs involve both fundamental research in nanomaterials, as well as specifically targeted systems of interest for energy and bio-environmental strategic areas.

FACILITIES

The following equipment and infrastructures are hosted and run at CFM by the different research groups:

CHEMICAL PHYSICS OF COMPLEX MATERIALS

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 Tunneling 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 (40K). Samples can be prepared independently at two different preparation chambers and they can be inserted in the instrument via a fast-entry lock.

SURFACE CHEMISTRY LAB

The "Surface Chemistry" laboratory is equipped with an Ultra High Vacuum chamber combining different surface characterization techniques: X-Ray Photoemission (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), Low Energy Electron Diffraction (LEED) and Scanning Tunneling Microscope (STM) (with the possibility to use it in Atomic Force Microscope (AFM) mode). The chamber has two sample preparation chambers, with the required Molecular Beam Epitaxy (MBE) and sample preparation tools.

SURFACE MAGNETISM LAB

The "Surface Magnetism" laboratory hosts equipment for surface characterization of samples by means of a homemade Magneto Optic Kerr Effect (MOKE, 15-300 K, 0.1 Tesla) and Scanning Tunneling Microscope (STM, Omicron, 70-800K). These two techniques can be used either combined or separately. The measuring ultra high vacuum chamber includes Low Energy Electron Diffraction (LEED) and Molecular Beam Epitaxy (MBE).

ULTRA-LOW TEMPERATURE SCANNING TUNNELING MICROSCOPY LAB

The "Ultra-Low Temperature Scanning Tunneling Microscopy" laboratory hosts an Atomic Force Microscopy (AFM) / Scanning Tunneling Microscope (STM) operable at 1K for characterization of materials at atomic scale.

ELECTRONIC PROPERTIES AT THE NANOSCALE

CERAMIC AND CEMENT-BASED MATERIALS LAB

The "Ceramic and Cement-based Materials" laboratory consists of the following specific equipment for synthesizing ceramics and cements:

- High temperature ceramic ovens (Thermolyne model from ThermoFisher Scientific)
- A high temperature microwave oven that features 3100 Watts of microwave power and controllable temperature up to 2000°C (BP-211/50 model from Microwave Research and Applications, Inc.)
- Homemade sub- and super-critical reactors

In the "Ceramic and Cement-based Materials" laboratory there is also an isothermal calorimeter (TAM Air 8-channel model from TA Instruments) for cements characterization.

LASER SPECTROSCOPY LAB

In the "Laser Spectroscopy" laboratory, continuous and time-resolved (with nano-picoseconds 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 characterize the properties of rare-earth-doped materials for lasing, spectral conversion, energy transfer and laser cooling. A homemade 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 picosecond (Infrared-Visible-Ultraviolet, IR VIS UV) and femtosecond (Infrared-Visible, IR-VIS) sources (with regenerative amplification) 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).

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.

Other available set-ups include:

- QUEPRO high-performance spectrophotometer connected to IX71 Olympus microscope for micro-photoluminescence spectroscopy
- Cary50 spectrophotometer (Agilent) for absorption and transmission spectroscopy
- Cary Eclipse Spectrophotometers (Agilent) for range of applications including photoluminescence and photoluminescence excitation spectroscopy, photoluminescence anisotropy spectroscopy, photoluminescence kinetics, phosphorescence and delayed fluorescence lifetime measurements
- Chemat KW4A precision spin-coater for deposition of thin organic and inorganic films from solutions and self-assembly of nanostructures

MATERIALS SYNTHESIS LAB

In the "Materials Synthesis" laboratory, materials' crystal growth is investigated by using homemade Bridgman and Czochralski furnaces. These facilities are physically located at the Engineering School of Bilbao (out of the CFM main premises in Donostia / San Sebastián).

QUANTUM NANOPHOTONICS LAB

The "Quantum Nanophotonics" laboratory is fully stabilized in temperature and humidity, and hosts state-of-the-art facilities for the generation and control of quantum states of light:

- Three optical tables for manipulating the polarization as well as spatial and frequency degrees of freedom of entangled and single photon states: 1200 x 2400 x 305 mm table with isolators (784-655-12DR model from TMC), 1500 x 3000 x 305 mm table with isolators (784-675-12DR model from TMC) and 900 x 1800 x 305 mm table with isolators (from Newport)
- A set of laser systems, including continuous wave lasers covering the ultra violet, visible and infrared regions, for producing different photon states: a 633nm, 10mW, He-Ne laser (from Thorlabs); a 403nm, 100mW, diode (from Toptica); a 680nm, 50mW, diode (from Toptica); a 808nm, 10mW, diode (from Thorlabs)
- Optically addressable cryostat, equipped with state-of-the-art nanopositioners, for cooling down nanostructures and nanoparticles to cryogenic temperatures (attoDRY 100 model from Attocube)
- A set of spatial light modulators (from Cambridge Correlators), polarizers (from Thorlabs and Standa) and Single Photon Counting Modules (SPCM, APDs SPCM-AQ4C model from Excelitas), for analyzing the photons interacting with nanostructures at cryogenic temperatures
- Microwave generators and amplifiers (SMB100A model from Rohde & Schwartz), for addressing the electronic states of Nitrogen Vacancy centers in diamond

POLYMERS AND SOFT MATTER

DIELECTRIC SPECTROSCOPY LAB

The "Dielectric Spectroscopy" laboratory provides characterization of dielectric properties of materials, particularly polymers and soft matter. 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
- Terahertz 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

MICROSCOPY LAB

The "Microscopy" laboratory allows structural characterization by means of:

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

CHEMISTRY LAB

The "Chemistry" laboratory is specialized in synthesis of polymers and soft matter based materials, with special focus on click chemistry methods. This laboratory can characterize physicochemical properties and stability of molecular and supramolecular chemical compounds using the following equipment:

- Absolute molecular mass distribution meter: Agilent 1200 GPC-SEC Analysis System + Wyatt. Light-scattering miniDAWN TREOS, viscosimetry ViscoStar II and Optilab rEX Refractive Index Detector
- Nanoparticle size and z-potential meter: Malvern Zetasizer Nano
- Viscometer: EMS-Viscometer EMS-1000 and 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 (200-550K, 0-27 bar)

THERMAL ANALYSIS LAB

The "Thermal Analysis" laboratory hosts the following equipment for material characterization, particularly polymers and soft matter:

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

MECHANICAL CHARACTERIZATION LAB

The "Mechanical Characterization" laboratory hosts the following equipment to perform rheological analysis in polymer and soft matter samples:

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

MOLECULAR SPECTROSCOPY LAB

The "Molecular Spectroscopy" laboratory hosts the following equipment to characterize solid and liquid samples, particularly polymers and soft matter:

- For the molecular spectroscopy in the infrared (IR) domain: FT-IR - JASCO 6300 (130-400K)
- For the molecular spectroscopy in the terahertz (THz) domain: TPS SPECTRA 3000, TeraView
- Raman scattering: FT-RAMAN, JASCO RFT-6000

X-RAY LAB

The "X-Ray" laboratory can provide characterization of polymer and soft matter samples by means of Small Angle X-Ray Scattering (SAXS) and Wide Angle X-Ray Scattering (WAXS) techniques (individually or simultaneously), using the following equipment:

- SAXS: Rigaku PSAXS-L (120-520K), which can operate with simultaneous WAXS measurements
- WAXS: Bruker AXS D8 ADVANCE (120-520K)

LIGHT SCATTERING LAB

The "Light Scattering" laboratory can provide characterization of polymer and soft matter samples by means of Static and Dynamic Light Scattering techniques (SLS and DLS, respectively), using a Light Scattering Spectrometer (288-363K) with modulated 3D technology.

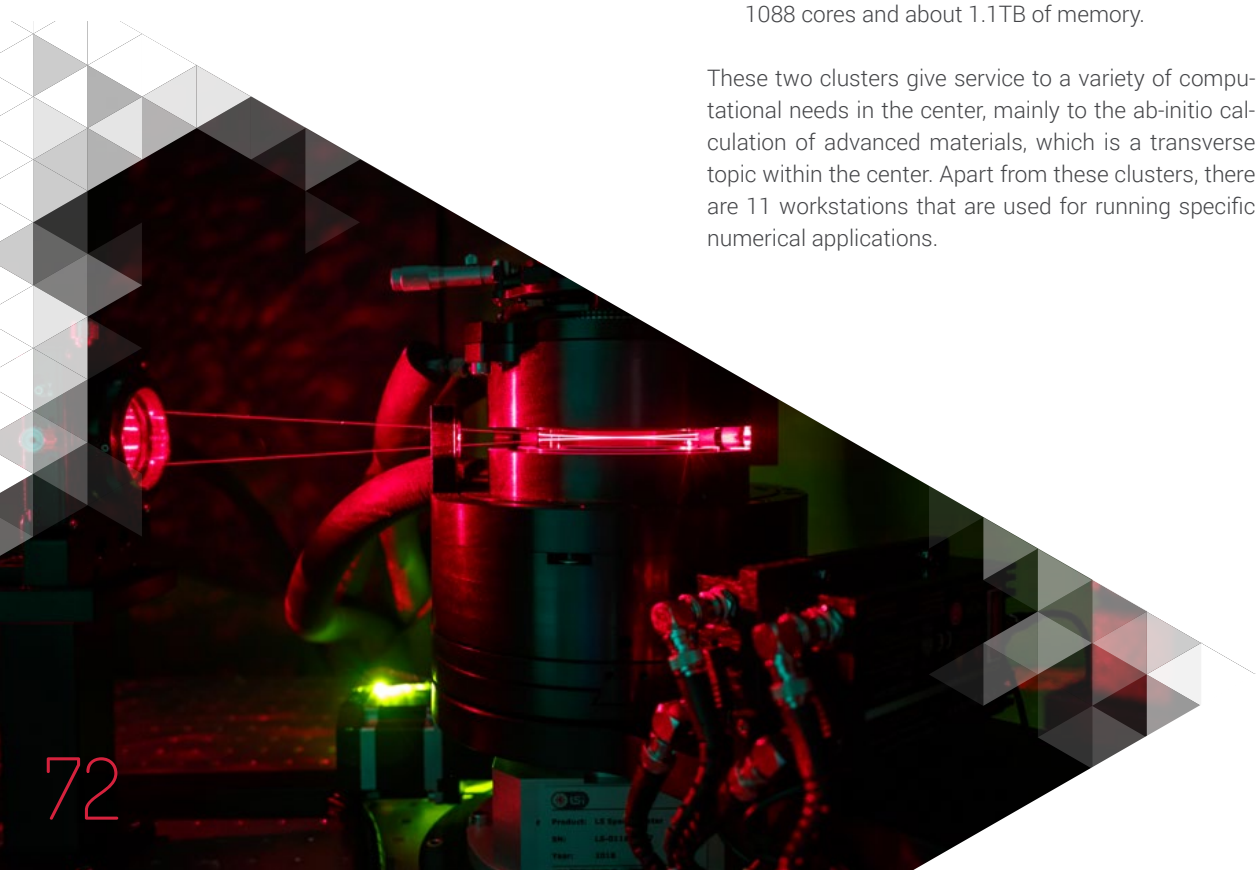
HIGH PERFORMANCE COMPUTING (HPC) CENTER

In addition to the experimental facilities, CFM has a Computing Center that provides scientific computing capabilities to the researchers of the center, giving a computing power of 45TFLOPS and a computing time of about 25.000.000 computing process unit (CPU) hours per year (about 3000 computing cores). It consists of two High Performance Computing (HPC) clusters:

- Oberon cluster (the main CFM HPC cluster) is composed of 182 computing nodes with two Xeon processors and a memory in the range of 24GB up to 256GB per node, all of them sharing a high speed-low latency Infiniband connection network and a high performance shared parallel filesystem, giving a total of around 1936 cores and 10TB 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 per node, giving a total of 1088 cores and about 1.1TB of memory.

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



EXTERNAL SERVICES

CFM offers external services based on the center's 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:

DIFFERENTIAL THERMAL ANALYSIS (DTA)

The service offers the thermal characterization of materials by means of differential scanning calorimetry technique, using a Flash Differential Scanning Calorimeter (180-700 K) from Mettler Toledo.

ISOBARIC THERMAL EXPANSION

The service offers the characterization of polymer and soft matter samples by means of dilatometry and PVT measuring system, using a L75V (100-800 K) from Linseis, and a pvT100 (200-550K, 200-2500 bar) from Thermo Haake, respectively.

ABSORPTION SPECTROSCOPY IN TERAHERTZ (THz) DOMAIN

The service offers the molecular characterization of samples by means of molecular spectroscopy in the THz domain, using a Terahertz spectrometer, TPS SPECTRA 3000 from TeraView.

DIELECTRIC CHARACTERIZATION

The service offers the characterization of dielectric properties of materials by means of a Broadband Dielectric Spectrometer (BDS) from ALPHA Novocontrol.

SMALL-ANGLE X-RAY DIFFRACTION

The service offers the structural characterization of materials by means of Small Angle X-Ray Scattering (SAXS) technique, using a Rigaku PSAXS-L (120-520K) SAXS instrument that enables simultaneous Wide Angle X-Ray Scattering (WASX) measurements.

MATERIALS SURFACE CHARACTERIZATION

The service offers the surface characterization of materials by means of X-Ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoemission Spectroscopy (UPS), Atomic Force Microscopy (AFM) and Scanning Tunneling microscopy (STM) techniques, either combined or separately.

NANOPHOTONICS LAB

The service offers time- resolved Photoluminescence (TRPL) measurements of materials using a MicroTime200 setup from PicoQuant that provides single molecule sensitivity and high temporal resolution.

RESEARCH OUTPUT

Among all the articles published at CFM, **76 %** were published in the framework of **international collaborations**, showing the international dimension and positioning of the Centre in the field of Materials Science.

14 % of these publications were developed as a result of joint work with research associations of international excellence such as the Max Planck Society as well as with 5 of the 10 best universities in the world according to the Shanghai Academic Ranking of World Universities (ARWU), in the area of natural sciences and mathematics (SCI). The list of such universities includes: University of California Berkeley, Stanford University, MIT (Massachusetts Institute of Technology), University of Cambridge and University of Tokyo.

ISI Publications in 2018
178

Q1 Publications in 2018
105

D1 Publications in 2018
63

H-index
118

ISI Web of Science citations*
11191

*As of March 2019
(Total number since 1999: 91787)

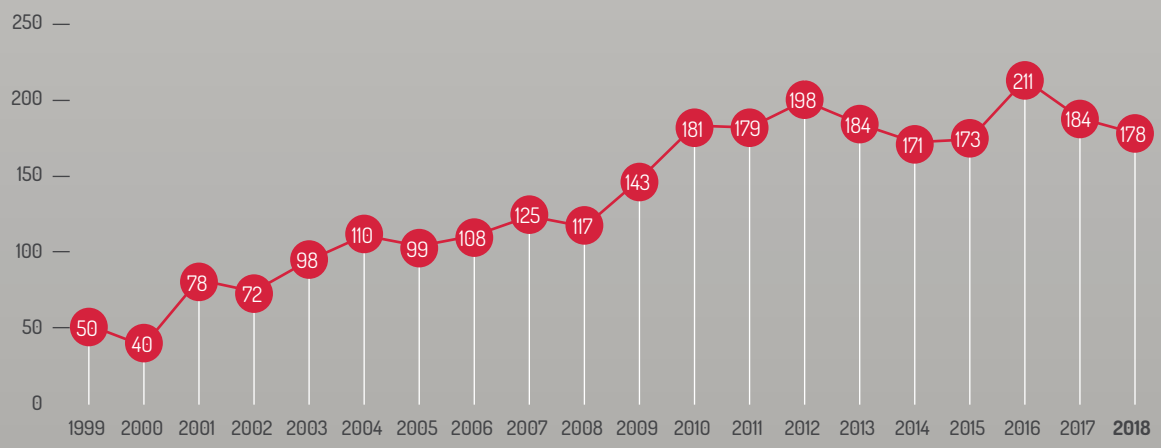
Average impact factor of the center in 2018
6.0

RESEARCH OUTPUT

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

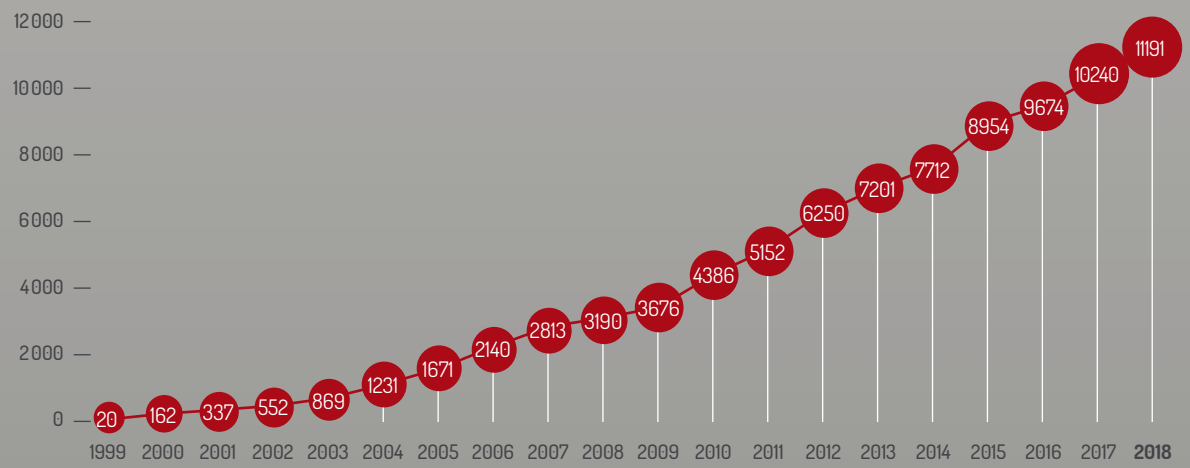
	2010	2011	2012	2013	2014	2015	2016	2017	**2018**
ISI PUBLICATIONS	181	179	198	184	171	173	211	184	**178**
Q1	134	144	149	139	131	129	178	116	**105**
D1	-	-	-	-	52	50	74	59	**63**

PUBLICATIONS



Total number of ISI publications since 1999 as of Arpil 2019: 2747

CITATIONS



Total number of ISI citations since 1999 as of April 2019: 91787

Total number of publications in and above Nano Research

Journal	Number of articles	Impact factor
Reviews of Modern Physics	1	36.37
Advanced Materials	3	21.95
Physical Review X	1	14.39
Journal of the American Chemical Society	2	14.36
ACS Nano	5	13.71
Light-Science & Applications	1	13.63
Advanced Functional Materials	1	13.33
Nature Communications	4	12.35
Nano Letters	5	12.08
Science Advances	1	11.51
Journal of Materials Chemistry A	1	9.93
Chemistry of Materials	1	9.89
Proceedings of the National Academy of Sciences of the United States of America	1	9.50
Chemical Science	1	9.06
Physical Review Letters	6	8.84
Journal of Physical Chemistry Letters	4	8.71
ACS Applied Materials & Interfaces	1	8.10
Nano Research	1	7.99

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1 **Controlling the Layer Localization of Gapless States in Bilayer Graphene with a Gate Voltage**
Jaskolski W, Pelc M, Bryant GW, Chico L, and Ayuela A.
2D Materials 5, 025006 (2018)

2 **Evidence of Large Spin-Orbit Coupling Effects in Quasi-Free-Standing Graphene on Pb/Ir(111)**
Otrokov MM, Klimovskikh II, Calleja F, Shikin AM, Vilkov O, Rybkin AG, Estyunin D, Muff S, Dil JH, de Parga ALV, Miranda R, Ochoa H, Guinea F, Cerda JI, Chulkov EV, and Arnau A.
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Bonardd S, Alegria A, Saldias C, Leiva A, and Kortaberria G.
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5 **Electronic Properties of Transferable Atomically Thin MoSe2/h-BN Heterostructures Grown on Rh(111)**
Chen MW, Kim H, Bernard C, Pizzochero M, Zaldivar J, Pascual JI, Ugeda MM, Yazyev OV, Greber T, Osterwalder J, Renault O, and Kis A.
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6 **Surface-Enhanced Molecular Electron Energy Loss Spectroscopy**
Konecna A, Neuman T, Aizpurua J, and Hillenbrand R.
ACS Nano 12, 4775 (2018)

7 **Chemical Mapping of Nanodefects within 2D Covalent Monolayers by Tip-Enhanced Raman Spectroscopy**
Shao F, Dai WY, Zhang Y, Zhang W, Schluter AD, and Zenobi R.
ACS Nano 12, 5021 (2018)

8 **Atomic-Scale Lightning Rod Effect in Plasmonic Picocavities: A Classical View to a Quantum Effect**
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9 **Photoactivation of Aggregation-Induced Emission Molecules for Fast and Efficient Synthesis of Highly Fluorescent Single-Chain Nanoparticles**
De-La-Cuesta J, and Pomposo, JA.
ACS Omega 3, 15193 (2018)

10 **Local Domain Size in Single-Chain Polymer Nanoparticles**
Pomposo JA, Moreno AJ, Arbe A, and Colmenero J.
ACS Omega 3, 8648 (2018)

11 **Special Issue on "Strong Coupling of Molecules to Cavities"**
Barnes B, Vidal FG, and Aizpurua J.
ACS Photonics 5, 1 (2018)

PUBLICATIONS

12 **Tailoring Multipolar Mie Scattering with Helicity and Angular Momentum**
Zambrana-Puyalto X, Vidal X, Wozniak P, Banzer P, and Molina-Terriza G.
ACS Photonics 5, 2936 (2018)

13 **All-Optical Self-Referenced Transverse Position Sensing with Subnanometer Precision**
Tischler N, Stark J, Zambrana-Puyalto X, Fernandez-Corbaton I, Vidal X, Molina-Terriza G, and Juan ML.
ACS Photonics 5, 3628 (2018)

14 **Metamaterial Platforms for Spintronic Modulation of Mid-Infrared Response under Very Weak Magnetic Field**
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15 **Doping as a Way to Protect Silicate Chains in Calcium Silicate Hydrates**
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16 **Hierarchical Aging Pathways and Reversible Fragile-to-Strong Transition upon Annealing of a Metallic Glass Former**
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18 **Chemically Responsive Elastomers Exhibiting Unity-Order Refractive Index Modulation**
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19 **When 2D Materials Meet Molecules: Opportunities and Challenges of Hybrid Organic/Inorganic van der Waals Heterostructures**
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20 **Vibrational Spectroscopy of Water with High Spatial Resolution**
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21 **Literature and Science. Towards an integration of knowledge**
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22 **Native and Graphene-Coated Flat and Stepped Surfaces of TiC**
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24 **Building a 22-Ring Nanographene by Combining in-Solution and on-Surface Syntheses**
Zuzak R, Castro-Esteban J, Brandimarte P, Engelund M, Cobas A, Piatkowski P, Kolmer M, Perez D, Guitian E, Szymonski M, Sanchez-Portal D, Godlewski S, and Pena D.
Chemical Communications 54, 10256 (2018)

25 **On-Surface Synthesis of Heptacene on Ag(001) from Brominated and Non-Brominated Tetrahydroheptacene Precursors**
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26 **Bias-Dependent Local Structure of Water Molecules at a Metallic Interface**
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27 **Synthesis, Crystal and Topological Electronic Structures of New Bismuth Tellurohalides Bi2TeBr and Bi3TeBr**
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28 **TCNQ Physisorption on the Topological Insulator Bi2Se3**
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Chemphyschem 19, 2405 (2018)

29 **Orbital-Selective Spin Excitation of a Magnetic Porphyrin**
Rubio-Verdu C, Sarasola A, Choi DJ, Majzik Z, Ebeling R, Calvo MR, Ugeda MM, Garcia-Lekue A, Sanchez-Portal D, and Pascual JI.
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30 **Influence of the Confinement Potential on the Size-Dependent Optical Response of Metallic Nanometric Particles**
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31 **Phase Evolution of KLaF4 Nanocrystals and their Effects on the Photoluminescence of Nd3+ doped transparent oxyfluoride glass-ceramics**
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De-La-Cuesta J, Asenjo-Sanz I, Latorre-Sanchez A, Gonzalez E, Martinez-Tong DE, and Pomposo JA.
European Polymer Journal 109, 447 (2018)

34 **Structural and Superconducting Properties of Tungsten Hydrides under High Pressure**
Zheng S, Zhang ST, Sun Y, Zhang J, Lin JY, Yang GC, and Bergara A.
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35 **80SiO(2)-20LaF(3) Oxyfluoride Glass Ceramic Coatings Doped With Nd3+ for Optical Applications**
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Zhou LS, Jiang B, Alducin M, and Guo H.
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40 **Effect of the Heat Treatment on the Spectroscopic Properties of Er3+-Yb3+-Doped Transparent Oxyfluoride Nano-Glass-Ceramics**
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41 **Transparent Oxyfluoride Glass-Ceramics with NaGdF4 Nanocrystals Doped with Pr3+ and Pr3+-Yb3+**
Velazquez JJ, Balda R, Fernandez J, Gorni G, Pascual L, Chen G, Sundararajan M, Duran A, and Pascual MJ
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42 **Interface Induced Quantized Spin Hall Response in Three-Dimensional Topological Insulator/Normal Insulator Heterostructures**
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Journal of Magnetism and Magnetic Materials 459, 231 (2018)

43 **Quantum Anomalous Hall Conductivity in 3D Magnetic Topological Insulator/Normal Insulator Heterostructures**
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44 **Sustainable Luminescent Solar Concentrators based on Organic-Inorganic Hybrids Modified with Chlorophyll**
Frias AR, Pecoraro E, Correia SFH, Minas LMG, Bastos AR, Garcia-Revilla S, Balda R, Ribeiro SJL, Andre PS, Carlos LD, and Ferreira RAS.
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45 **Active Quinine-Based Films Able to Release Antimicrobial Compounds via Melt Quaternization at Low Temperature**
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46 **The Maximum Positive Curvature Recognition Method to Determine Etch Profiles in Wet Etching of Quartz on AT and BT Cuts**
Xing Y, Zhang J, Gosalvez MA, Zhang H, Li Y, and Zhou SH.
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47 **Transparent Glass-Ceramics of Sodium Lutetium Fluoride Co-Doped with Erbium and Ytterbium**
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48 **Roadmap on Plasmonics**
Stockman MI, Kneipp K, Bozhevolnyi SI, Saha S, Dutta A, Ndukaife J, Kinsey N, Reddy H, Guler U, Shalaev VM, Boltasseva A, Gholipour B, Krishnamoorthy HNS, MacDonald KF, Soci C, Zheludev NI, Savinov V, Singh R, Gross P, Lienau C, Vadai M, Solomon ML, Barton DR, Lawrence M, Dionne JA, Boriskina SV, Esteban R, Aizpurua J, Zhang X, Yang S, Wang DQ, Wang WJ, Odom TW, Accanto N, de Roque PM, Hancu IM, Piatkowski L, van Hulst NF, and Kling MF.
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49 **A Definition of the Magnetic Transition Temperature Using Valence Bond Theory**
Jornet-Somoza J, Deumal M, Borge J, and Robb MA.
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50 **Star Block-Copolymers in Shear Flow**
Jaramillo-Cano D, Formanek M, Likos CN, and Camargo M.
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51 **Nonmetallic FeH6 under High Pressure**
Zhang ST, Lin JY, Wang YC, Yang GC, Bergara A, and Ma YM.
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52 **Electronic Properties of Substitutionally Boron-Doped Graphene Nanoribbons on a Au(111) Surface**
Carbonell-Sanroma E, Garcia-Lekue A, Corso M, Vasseur G, Brandimarte P, Lobo-Checa J, de Oteyza DG, Li JC, Kawai S, Saito S, Yamaguchi S, Ortega JE, Sanchez-Portal D, and Pascual JI.
Journal of Physical Chemistry C 122, 16092 (2018)

53 **Inelastic Scattering of N-2 off W(001): Reconciling Experiment and Theory at Low Collision Energies**
Ibarguen C, Larregaray P, Pena-Torres A, and Crespos C.
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PUBLICATIONS

54 **Electron-Phonon Interaction in the 4/3-Monolayer of Pb on Si(111): Theory Versus He-Atom Scattering Experiments**
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Journal of Physical Chemistry C 122, 29039 (2018)

55 **Effect of Structural Fluctuations on Elastic Lifetimes of Adsorbate States: Isonicotinic Acid on Rutile(110)**
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56 **Tracing Polymerization in Calcium Silicate Hydrates Using Si Isotopic Fractionation**
Dupuis R, Dolado JS, Surga J, and Ayuela A.
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57 **Unraveling the Electronic Structure of Narrow Atomically Precise Chiral Graphene Nanoribbons**
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58 **Switching from Reactant to Substrate Engineering in the Selective Synthesis of Graphene Nanoribbons**
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59 **Room-Temperature Optical Picocavities below 1 nm(3) Accessing Single-Atom Geometries**
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60 **Direct Calorimetric Observation of the Rigid Amorphous Fraction in a Semiconducting Polymer**
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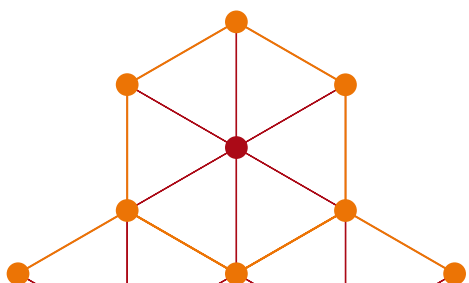

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Carbonell-Sanroma E, Corso M, Li JC, Brion-Rios AX, Sanchez-Portal D, and Pascual JI.
Surface Science 678, 189 (2018)

171 **Tunneling Electronic Currents Simulated with Localized Basis Sets**
Garcia-Fernandez C, and Lorente N.
Surface Science 678, 201 (2018)

172 **Phonons and Electron-Phonon Anomalies in Ultra-Thin Pb Films on Si(111) and Ge(111)**
Benedek G, Sklyadneva IY, Chulkov EV, Echenique PM, Heid R, Bohnen KP, Schmicker D, Schmidt S, and Toennies JP.
Surface Science 678, 38 (2018)

PUBLICATIONS

173 **Dynamics and Mean-Free Path of Electronic Excitations in WSe2**
Silkin VM, Krasovskii EE, Chulkov EV, and Echenique PM.
Surface Science 678, 72 (2018)

174 **Phonon-Induced Linewidth of Quantum-Well States in Monolayer Pb on Si(111)**
Sklyadneva IY, Heid R, Bohnen KP, and Chulkov EV.
Surface Science 678, 86 (2018)

175 **Electronic and Crystal Structure of the Pt(111)-(root 3 x root 3)R30 Degrees-K System**
Koroteev YM, and Chulkov EV.
Surface Science 678, 99 (2018)

176 **Notable Reactivity of Acetonitrile towards Li2O2/LiO2 Probed by NAP XPS during Li-O-2 Battery Discharge**
Zakharchenko TK, Belova AI, Frolov AS, Kapitanova OO, Velasco-Velez JJ, Knop-Gericke A, Vyalikh D, Itkis DM, and Yashina LV.
Topics in Catalysis 61, 2114 (2018)

177 **Analysis of Electromagnetic Forces and Causality in Electron Microscopy**
Reyes-Coronado A, Ortiz-Solano CG, Zabala N, Rivacoba A, and Esquivel-Sirvent R. Ultramicroscopy 192, 80 (2018)

178 **Energy Transfer between Single Semiconductor Quantum Dots and Organic Dye Molecules**
Melnikau D, Hendel T, Linkov PA, Samokhvalov PS, Nabiev IR, and Rakovich YP.
Zeitschrift Fur Physikalische Chemie- International Journal of research in Physical Chemistry & Chemical Physics 232, 1513 (2018)

BOOK CHAPTERS

Relaxation Processes in Liquids and Glass-Forming Systems: What Can We Learn by Comparing Neutron Scattering and Dielectric Spectroscopy Results?

Arbe A, and Colmenero J.

The Scaling of Relaxation Processes (2018) 247-277. Springer

Magnetic Impurities on Surfaces: Kondo and Inelastic Scattering

Choi DJ, and Lorente N.

In: Andreoni W., Yip S. (eds) Handbook of Materials Modeling (2018) 1-32. Springer, Cham

Physical Aging of Polymers

Cangialosi D.

Encyclopedia of Polymer Science and Technology (2018) John Wiley & Sons, Inc.

Glass Transition and Physical Aging of Confined Polymers Investigated by Calorimetric Techniques

Cangialosi D.

Handbook of Thermal Analysis and Calorimetry 6, (2018) 301-337. Elsevier

TRAINING ACTIVITIES

As a joint center 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.

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.

PHD PROGRAM: PHYSICS OF NANOSTRUCTURES AND ADVANCED MATERIALS

"Physics of Nanostructures and Advanced Materials" is a PhD program of UPV/EHU that has been recognized 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 center.
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.

PHD THESES DEFENDED AT CFM IN 2018

- **Chain dynamics in crosslinked filled and unfilled polymer blends of different miscibility**
  Author: Lucia Ortega
  Supervisors: Silvina Cerveny and Gustavo A. Schwartz
  Group: Polymers and Soft Matter
  16/03/2018

- **Non-adiabatic processes in the radiation damage of materials from first-principles**
  Author: Rafi Ullah
  Supervisors: Emilio Artacho and Daniel Sánchez-Portal
  Group: Modelisation and Simulation
  23/03/2018

- **Non-equilibrium dynamics and molecular mobility in polymer glasses: From bulk to 3-D confinement**
  Author: Natalia Gutiérrez
  Supervisor: Daniele Cangialosi
  Group: Polymers and Soft Matter
  25/05/2018

- **Plasmons in nanoparticles: Atomistic ab initio theory for large systems**
  Author: Marc Barbry
  Supervisors: Peter Koval and Daniel Sánchez-Portal
  Group: Modelisation and Simulation
  05/07/2018

- **Hydrogen and lithium under high pressure. Superconductivity and other emerging properties**
  Author: Miguel Borinaga
  Supervisors: Aitor Bergara and Ion Errea
  Group: Materials Computation and Theory
  06/07/2018

- **Theoretical study of the linear and nonlinear optical response of plasmonic tunneling gaps**
  Author: Garikoitz Aguirregabiria
  Supervisors: Rubén Esteban and Javier Aizpurua
  Group: Theory of Nanophotonics
  07/09/2018

- **Theoretical studies on molecular adsorption and the effect of strain on core-level spectroscopy in different metal surfaces**
  Author: Antón X. Brión
  Supervisors: Pepa Cabrera-Sanfelix and Daniel Sánchez-Portal
  Group: Modelisation and Simulation
  15/10/2018

- **Electronic bands of nanoporous networks and one-dimensional covalent polymers assembled on metal surfaces**
  Author: Ignacio Piquero
  Supervisors: Jorge Lobo and Enrique Ortega
  Group: Nanophysics Lab
  30/11/2018

- **Contribution to the theoretical description of N2 dynamics on W(100)**
  Author: Cédric Crespos
  Supervisor: Iñaki Juaristi
  Group: Gas/Solid Interfaces
  10/12/2018

- **Theory of plasmon-enhanced spectroscopy of molecular excitations: infrared absorption, fluorescence, and Raman scattering**
  Author: Tomas Newman
  Supervisor: Javier Aizpurua
  Group: Theory of Nanophotonics
  14/12/2018

SHORT STAYS IN FOREIGN UNIVERSITIES

A very important aspect of the PhD training program consists of supporting short stays in foreign universities and centers for PhD students. An average of about 6 PhD students per year spend about 2-3 months in some of the best international centers on their topics. This training activity combines aspects of internationalization and excellence, and has been strongly supported within the last years by CFM. The following pre-doctoral researchers benefited from an internship abroad supported by CFM in 2018:

- **Andrea Konečná**
  Oak Ridge National Laboratory (Tennessee, USA)
  1 April - 1 June
- **Maud Formanek**
  Universitá di Roma "La Sapienza" (Italy)
  3 May - 5 July
- **Thomas Gambino**
  Center Clermont-Ferrand (France)
  3 June - 28 July
- **Antton Babaze**
  Institute of Sciences Moleculaires de Orsay (ISMO) (France)
  28 May - 28 June

MASTER IN NANOSCIENCE

Master in Nanoscience is an official Master program of UPV/EHU (held at CFM headquarters) and co-organized 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 center 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, the students choose to develop the skills either in fields directly linked with applied and technology-oriented research work in technological centers, or in the basic/oriented research that is carried out in academic research groups. The students will also be able to start developing the research work that may allow them to access the PhD program.

MASTER THESES SUCCESSFULLY DEFENDED AT CFM IN 2018

- **Structural and electronic properties of metal hosted porphyrins and phthalocyanines on Au(111) and GdAu2 /Au(111)**
  Author: Rodrigo Castrillo
  Supervisor: Frederik M. Schiller

- **Characterization of surface ruthenium oxides with catalytic interest**
  Author: José Enrique Barranco
  Supervisors: Sara Barja and Celia Rogero

- **Polaritons in biaxial crystals**
  Author: Gonzalo Álvarez
  Supervisors: Alexey Nikitin and Pablo Alonso González

- **Nanostructured transducers for enhanced plasmonic biosensing**
  Author: Leire Fernández
  Supervisors: María Carmen Morant-Miñana and Andreas Seifert

- **Spin-dependent transport in diffusive systems with intrinsic spin-orbit coupling**
  Author: Ricardo Rama
  Supervisor: F. Sebastián Bergeret

- **Field-enhanced CD spectroscopy with subwavelength silicon particle arrays**
  Author: Jon Lasa
  Supervisors: Javier Aizpurua and Aitzol García-Etxarri

- **Characterization of the magnetic properties of the herringbone lattice**
  Author: Miguel Ángel Jiménez
  Supervisor: Dario Bercioux

- **VPI-based induction of conductivity into Kevlar fibers**
  Author: Gabriele Botta
  Supervisors: Mato Knez and Itxasne Azpitarte Iraculis

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.

In the framework of this teaching activity, undergraduate students can join a research group at CFM for a short stay or to fulfill their End of Course Project during the academic year.

HOSTED STUDENT TRAINING

- **Celia González Sánchez (short visiting)**
  Supervisor: Frederik M. Schiller
  Group: Nanophysics Lab

- **Ander Arregui Biera**
  Supervisor: Celia Rogero
  Group: Nanophysics Lab

- **Irati Garmendia San Miguel**
  Supervisor: Celia Rogero
  Group: Nanophysics Lab

- **Ane Telleria Lazcano**
  Supervisor: Celia Rogero
  Group: Nanophysics Lab

END OF COURSE PROJECTS DEFENDED

Out of all trainings, four students defended their End of Course Project during 2018:

- **Síntesis de nanopartículas poliméricas unimoleculares fluorescentes**
  Author: Julen Gorospe
  Supervisor: Josetxo Pomposo
  Group: Polymers and Soft Matter

- **Tiolación de polietilenglicol para la funcionalización de nanopartículas de oro**
  Author: Pedro Liz
  Supervisor: Fabienne Barroso
  Group: Polymers and Soft Matter

- **Síntesis de nanopartículas pliméricas unimoleculares para dosificación controlada**
  Author: Jokin Pinacho
  Supervisor: Josetxo Pomposo
  Group: Polymers and Soft Matter

- **Analysis of entangled photon pair configurations for bright optical sources**
  Author: Evan Villafranca
  Supervisor: Gabriel Molina
  Group: Quantum Nanophotonics Laboratory

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 hosted five summer internships for undergraduate students during 2018, three of them being supported by MPC grants and two by DIPC:

- **Guillermo Hijano**
  Supervisor: Celia Rogero
  Group: Nanophysics Lab

- **Tatiana Nidybeth Claros**
  Supervisor: Josetxo Pomposo
  Group: Polymers and Soft Matter

- **Unai Arregui**
  Supervisor: Rubén Esteban
  Group: Theory of Nanophotonics

- **Mikel Dolz**
  Supervisor: Fabienne Barroso
  Group: Polymers and Soft Matter

- **Alberto Hijano**
  Supervisor: F. Sebastián Bergeret
  Group: Mesoscopic Physics

OTHER TRAINING COURSES

CFM administration organizes health and safety security courses given by CSIC and UPV/EHU central services, as well as IT courses (Software Carpentry) given by the Computing Service Manager, or external experts (COMSOL).

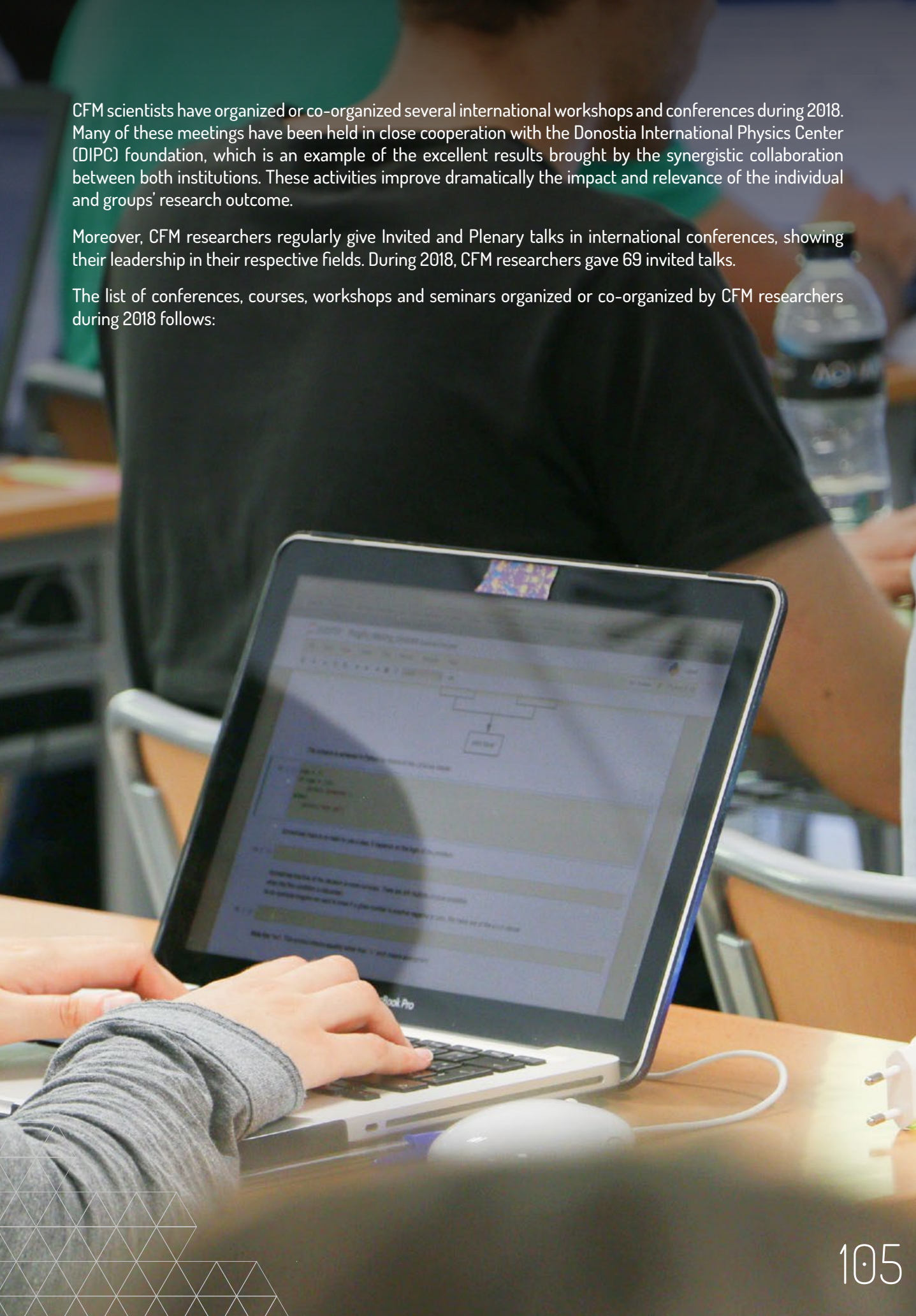
Other specialized courses about specific experimental techniques are also organized. Furthermore, a laboratory course on dielectric spectroscopy is successfully organized by CFM researcher Prof. Ángel Alegría, in which 15-20 graduate students and researchers take part yearly.

WORKSHOPS, CONFERENCES AND SEMINARS

CFM scientists have organized or co-organized several international workshops and conferences during 2018. Many of these meetings have been held in close cooperation with the Donostia International Physics Center (DIPC) foundation, which is an example of the excellent results brought by the synergistic collaboration between both institutions. These activities improve dramatically the impact and relevance of the individual and groups' research outcome.

Moreover, CFM researchers regularly give Invited and Plenary talks in international conferences, showing their leadership in their respective fields. During 2018, CFM researchers gave 69 invited talks.

The list of conferences, courses, workshops and seminars organized or co-organized by CFM researchers during 2018 follows:



INTERNATIONAL CONFERENCES

Functional Polymers

Juan Colmenero (Chair; CFM, and UPV/EHU), Dieter Richter (Chair; Jülich Center for Neutron Science), Josetxo Pomposo (CFM, and UPV/EHU), Angel Moreno (CFM, and CSIC) and Arantxa Arbe (CFM, and CSIC)
DIPC, Donostia / San Sebastián
19 - 21/03/2018

HIGHper2018- International Spring School on High Performance Computing

Iñigo Aldazabal (Co-chair; CFM), Carlos Martín-Vide (Co-chair), Manuel J. Parra-Royón (CERN, Switzerland), Txomin Romero (Co-chair; DIPC) and David Silva (Institute for Research Development, Training and Advice, IRDTA, Belgium)
Centro Ignacio María Barriola (UPV/EHU), Donostia / San Sebastián
23 - 27/04/2018

Euskal Esperientziak Zientzia Zabalkuntzan (EEZZ18)

Amaia Arregi (DIPC), Uxune Martinez (UPV/EHUko Kultura Zientifikoko Katedra, KZK), Jon M. Matxain (UPV/EHU, and DIPC), and Idoia Mugica (CFM)
Carlos Santamaría Center (UPV/EHU), Donostia / San Sebastián
14 - 15/06/2018

Novel 2D Materials Explored via Scanning Probe Microscopy & Spectroscopy
Miguel Moreno (CFM, and DIPC) and Iván Brihuega (IFIMAC, and UAM)
Miramar Royal Palace, Donostia / San Sebastián
25 - 30/06/2018

Quantum Designer Physics

Daniel Loss (University of Basel, Switzerland), Francisco Guinea (IMDEA Nanoscience, and University of Manchester, UK), Andres Arnau (CFM, UPV/EHU, and DIPC) and Vitaly Golovach (CFM, and DIPC)
Miramar Royal Palace, Donostia / San Sebastián
16 - 18/07/2018

New Generation in Strongly Correlated Electrons Systems

Santiago Blanco-Canosa (CIC nanoGUNE, and DIPC), George Booth (King´s College, UK), Wojciech Brzezicki (International Research Centre MagTop, Poland), Ion Errea (CFM, UPV/EHU, and DIPC), Matteo Minola (Max Planck Institute for Solid State Research, Germany) and Laurenz Rettig (Fritz Haber Institute, Germany)
Miramar Royal Palace, Donostia / San Sebastián
3 - 7/09/2018

The Second Spins on Surfaces (SoS II)

Deung-Jang Choi (CFM, and DIPC) and Andreas Heinrich (DIPC, and UPV/EHU)
Miramar Royal Palace, Donostia / San Sebastián
10 - 14/09/2018

Spanish Conference on Nanophotonics (CEN2018)

Javier Aizpurua (CFM, and DIPC), Luis Liz-Marzán (CIC biomaGUNE), Rubén Esteban (DIPC), Gabriel Molina-Terriza (CFM, UPV/EHU, and CSIC), Rainer Hillenbrand (CIC nanoGUNE), Aitzol García-Etxarri (Chair; DIPC), and Juan José Sáenz (Chair; DIPC)
Carlos Santamaría Center (UPV/EHU), Donostia / San Sebastián
3 - 5/10/2018

COURSES

Simulation Approaches for Building Materials (Master Course)

Jorge Sánchez-Dolado
University of Cádiz, Cádiz
25 - 26/09/2018

RILEM Multiscale Modelling Course for Concrete (MMC2)

Jorge Sánchez-Dolado
Delft University of Technology, Delft, The Netherlands
2 - 6/10/2018

8th Laboratory Course on Dielectric Spectroscopy

Ángel Alegría (CFM), Silvia Arrese-Igor (CFM), Daniele Cangialosi (CFM), Silvina Cerveny (CFM), and Gustavo A. Schwartz (CFM) in collaboration with DIPC, and UPV/EHU Vice-rectorate of the campus of Gipuzkoa
CFM, Donostia / San Sebastián
7 - 11/05/2018

WORKSHOPS

Transborder QuantumChemPhys Lab Workshop

Ricardo Díez-Muiño (CFM, and DIPC) and Pascal Larregaray *(Université de Bordeaux,* France)
Baiona, France
5 - 6/11/2018

Software Carpentry Workshop

Iñigo Aldazabal, the computing service manager at CFM, is a certified software and data carpentry instructor, and yearly organizes a series of workshops related to the field in different locations:

Lund, Sweeden

Iñigo Aldazabal (CFM, CSIC-UPV/EHU) and Andrés Díaz-Gil *(Instituto de Física Teórica,* IFT)
15 - 16/03/2018

Donostia / San Sebastián

Iñigo Aldazabal (CFM, CSIC-UPV/EHU), Andrés Diaz-Gil (Institute for Theoretical Physics, UAM-CSIC, Madrid), David de Sancho (CIC nanoGUNE), Anita C. Schürch (University Medical Center Utrech, The Netherlands)
27 - 29/06/2018

Madrid

Iñigo Aldazabal (CFM, CSIC-UPV/EHU), Francisco J. Martínez-Murcia *(Universidad de Granada),* Bryan Zaldivar *(Instituto de Física Teórica,* IFT, CSIC, and UAM), and Alfonso Nuñez *(Instituto de Ciencias Matemáticas,* ICM, CSIC, and UAM), and Emilio Ambite (IFT, CSIC, and UAM), Eduardo de Córdoba (ICM, CSIC-UAM), Andrés Díaz-Gil (CSIC, and UAM), David Gordo (IFT, CSIC, and UAM), and Marcos Ramírez (IFT, CSIC, and UAM) as helpers
28 - 30/11/2018

Donostia / San Sebastián

Iñigo Aldazabal (CFM, CSIC-UPV/EHU), David de Sancho (DIPC), Sofía Sanz (DIPC), and Daniel J. Arismendi (DIPC), and Xiang Xu (DIPC) as helpers
5, 10, 13, 18, and 19/12/2018

PHD SEMINAR SERIES

Since 2013, a regular series of seminars delivered by PhD students is organized at CFM. This activity continued during 2018. Approximately every two weeks, from September to June, two PhD students present updated results of their respective theses 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 2018 follows:

- **Strong electron-phonon and band structure effects in the optical properties of high pressure metallic hydrogen**
  Miguel Borinaga
  07/02/2018

- **Dynamics of N2 scattering on W(100) including van der Waals interactions: Energy dissipation effects**
  Alejandro Peña
  07/02/2018

- **Second order structural phase transition, spectral function and thermal conductivity of thermoelectric SnSe**
  Unai Aseguinolaza
  28/02/2018

- **Magnetic properties from multiplet calculations**
  Iker Gallardo
  07/03/2018

- **Electron refrigeration in hybrid structures with spin-split superconductors**
  Mikel Rouco
  07/03/2018

- **Separation of the Coulomb hole into weak and strong correlation contributions**
  Mireia Via-Nadal
  11/04/2018

- **Edge states in chiral-shaped graphene nanoribbons**
  Nestor Merino
  11/04/2018

- **Structure and electronic properties of dibromo benzothiadiazole on Cu(110)**
  Ana Barragán
  25/04/2018

- **Localizing the angular momentum of light at the nanoscale**
  Mattin Urbieta
  25/04/2018

- **Non-uniform superconducting phases generated by spin-orbit interaction**
  Julie Baumard
  09/05/2018

- **Suppression of the Hanle effect by coupling to valley polarized currents**
  Xiangpeng Zhang
  09/05/2018

MORE SEMINARS HELD AT CFM

- **Surfaces and interfaces in organic bulk-heterojunction solar cells**
  S. Ismat Shah
  23/01/2018

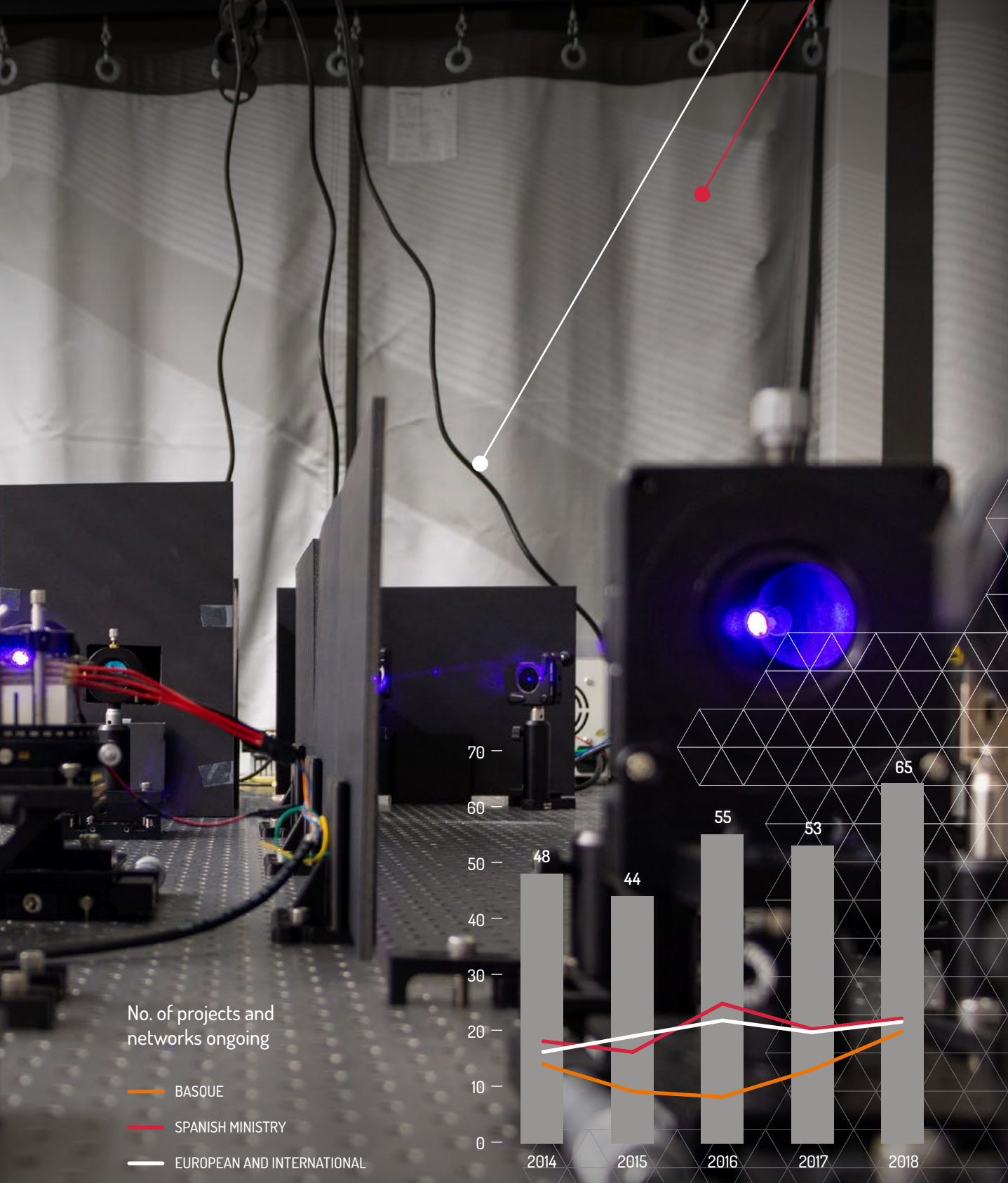
- **What does Outreach stand for at CFM? Introducing the Outreach Plan 2018**
  Idoia Mugica
  04/07/2018

- **Job in industry after the PhD**
  Marc Barbry
  08/11/2018

- **Pulsed neutrons for materials discovery**
  Felix Fernandez-Alonso
  12/11/2018

COMPETITIVE FUNDING FOR RESEARCH PROJECTS

Funding approved in 2018	
BASQUE RESEARCH PROJECTS	663 081.69 €
SPANISH MINISTRY RESEARCH PROJECTS	863 597.45 €
EUROPEAN AND INTERNATIONAL PROJECTS AND NETWORKS	1 041 340.41 €
MPC-BERC	1 243 560.00€
TOTAL	**3 811 579.55 €**



The projects that were in progress during 2018 (a total of 65 projects) are listed in the following, according to the source of competitive funding.

BASQUE RESEARCH PROJECTS

- **EJ/GV, IKERTALDE 2013, Grupo Consolidado IT578-13**
  Energy Materials: Fundamental developments in AB-initio computational material science
  PI: Ángel Rubio Secades

- **EJ/GV, IKERTALDE 2013, Grupo Consolidado IT621-13**
  Física de nanoestructuras experimental
  PI: Enrique Ortega Conejero

- **EJ/GV, IKERTALDE 2013, Grupo Consolidado IT654-13**
  Polímeros y materia condensada blanda
  PI: Juan Colmenero de León

- **EJ/GV, IKERTALDE 2013, Grupo Consolidado IT756-13**
  Estudio teórico de propiedades estructurales y electrónicas de nanoestructuras y superficies
  PI: Andrés Arnau Pino

- **EJ/GV, IKERTALDE 2016, Grupo Consolidado IT943-16**
  Grupo de Espectroscopía Láser y Materiales Fotónicos
  PI: Rolindes Balda de la Cruz

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

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

- **EJ/GV, ELKARTEK 2018, KK-2018/00001**
  nG8 - Investigación Colaborativa para la Caracterización Avanzada de Sistemas Macroscópicos en la Nanoescala
  PI: Javier Aizpurua Iriazabal

- **EJ/GV, Proyectos de Investigación Básica y/o Aplicada 2018-2020 (PIBA), PIBA18-24**
  Diseño, elaboración y caracterización de materiales nano-micro estructurados ópticamente activos en el rango visible e infrarrojo próximo para la construcción de una fuente láser aleatoria de baja coherencia para aplicaciones biomédicas
  PI: Rolindes Balda de la Cruz

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, RED2017, 2017-CIEN-000085-01**
  Desarrollo del laboratorio de nanoóptica cuántica
  PI: Gabriel Molina Terriza

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, RED2017, 2017-CIEN-000083-01**
  Desarrollo de nanopartículas de Povidona para dosificación de fármacos anticancerosos con detección por fluorescencia
  PI: Josetxo Pomposo Alonso

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa Coopera 2017, 2017 IZEN-000013-01**
  Fortalecimiento instrumental del laboratorio de caracterización óptica de materiales a crearse en la Universidad Distrital Francisco José de Caldas

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Fellows Gipuzkoa 2017, 2017 FELL-000006-01**
  Síntesis de nanopatículas poliméricas unimoleculares altamente fluorescentes para aplicaciones en bioimagen
  Supervisor: Josetxo Pomposo Alonso

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, RED2018, 2018-CIEN-000025-01**
  INTERFACES - Interfaces de aislantes topológicos
  PI: Lucia Vitali

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, RED2018, 2018-CIEN-000036-01**
  Fuente de plasma para crecimiento de nuevos materiales funcionales en condiciones de ultra alto vacío
  PI: Sara Barja Martínez

BASQUE RESEARCH PROJECTS

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa Coopera 2018, 2018 IZEN-000013**
  Ellas Investigan

- **UPV/EHU, Azpiegitura zientifikoa/Infraestructura científica, INF 17/08**
  Renovación de un analizador dieléctrico de banda ancha
  PI: Juan Colmenero de León

- **UPV/EHU, Ikerketa Taldeak / Grupos de Investigación UPV/EHU 2017, GIU17/014**
  Grupo de Espectroscopía Láser y Materiales Fotónicos
  PI: Rolindes Balda de la Cruz

- **UPV/EHU, Ikerketa Taldeak / Grupos de Investigación UPV/EHU 2018, GIU18/202**
  PASMOACTIV - Nanoplasmónica activa para el desarrollo de dispositivos optoelectrónicos, sensores ópticos, espectroscopía de campo cercano y nanoscopías
  PI: Javier Aizpurua Irizabal
  Co-PI: Nerea Zabala Unzalu

- **UPV/EHU, Ikerketa Taldeak / Grupos de Investigación UPV/EHU 2018, GIU18/209**
  Nanophyscis Lab San Sebastián: desde la ciencia de superficies a los dispositivos
  PI: Enrique Ortega Conejero
  Co-PI: Martina Corso

SPANISH MINISTRY RESEARCH PROJECTS

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2014, FIS2014-55987-P**
  Transporte de espín en estructuras hibridas: metales. Superconductores, semiconductores, grafeno y aislantes topológicos
  PI: F. Sebastián Bergeret Sbarbaro

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2015, MAT2015-63704-P**
  De las nano-partículas blandas unimoleculares a los nano-compuestos totalmente poliméricos
  PI: Juan Colmenero de León

- **MEC-MICINN, Retos Investigación 2015, MAT2015-66888-C3-2-R**
  Magnetismo en la nanoescala: explorando nuevas rutas (Física de dispositivos de spin)
  PI: Nicolás Lorente Palacios

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

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2016, FIS2016-75862-P**
  Propiedades estructurales, electrónicas y magnéticas de sistemas en escala nanométrica
  PI: Andrés Arnau Pino

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2016, FIS2016-76471-P**
  Transferencia de energía en la interacción y dinámica de átomos y moléculas en superficies
  PI: Ricardo Diez Muiño
  Co-PI: Maite Alducin Ochoa

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2016, FIS2016-76617-P**
  Excitaciones electrónicas en superficies y nanoestructuras
  PI: Andrés Ayuela Fernández

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2016, FIS2016-79464-P**
  SElecT-DFT – Transporte Electrónico, Térmico, y de Espín con la Teoría de Funcionales de Densidad
  PI: Ángel Rubio Secades

SPANISH MINISTRY RESEARCH PROJECTS

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2016, FIS2016-80174-P**
  Nanoplasmónica cuántica para el desarrollo del control activo en optoelectrónica, las espectroscopias aumentadas por campo y la nanoscopia
  PI: Javier Aizpurua Iriazabal

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2016, FIS2016-77188-P**
  Teoría y simulación de fenómenos ópticos y de transporte en materiales girotrópicos
  PI: Ivo Souza

- **MEC-MICINN, Retos Investigación 2016, MAT2016-78293-C6-4-R**
  Teoría de nanoestructuras moleculares funcionales para dispositivos optoelectrónicos
  PI: Daniel Sánchez Portal

- **MEC-MICINN, Retos Investigación 2016, MAT2016-78293-C6-5-R**
  Nanoestructuras moleculares funcionales para dispositivos optoelectrónicos: Guiando reacciones en superficies
  PI: Celia Rogero Blanco

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

- **MEC-MICINN, Redes de Excelencia 2016, FIS2016-81977-REDC**
  RedLUR – Red Española de Láseres Ultrarrápidos
  PI: Rolindes Balda de la Cruz

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2017, FIS2017-82804-P**
  Transporte electrónico en estructuras híbridas: materiales de baja dimensionalidad, superconductores, materiales magnéticos, semiconductores y metales normales
  PI: F. Sebastián Bergeret Sbarbaro

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2017, FIS2017-87363-P**
  Nanofotónica cuántica: explorando las correlaciones cuánticas de los fotones usando nanopartículas
  PI: Gabriel Molina Terriza

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2017, MAT2017-88374-P**
  Magnetismo exótico y fenómenos de correlación de electrones en la superficie y el sólido de materiales basadas en tierras raras
  PI: Frederik M. Schiller

- **MEC-MICINN, Proyectos I+D Fundamental (Excelencia) 2017, MAT2017-87035-C2-2-P**
  Vidrios y vitrocerámicos dopados con tierras raras para aplicaciones fotónicas
  PI: Rolindes Balda de la Cruz

- **MEC-MICINN, Retos Investigación 2017, MAT2017-88377-C2-2-R**
  Transistores de spin basados en heteroestructuras van der Waals
  PI: Sara Barja Martínez

- **MEC-MICINN, Redes de Excelencia 2017, MAT2017-90771-REDT**
  ESpín - Red: Red Española de Espintrónica
  Partner: Andrés Arnau Pino

- **MEC-MICINN, Adquisición de Equipamiento Científico-Técnico 2018, EQC2018-004060-P**
  Plataforma de pinzas ópticas para el estudio de sensores cuánticos aplicados a biología
  PI: Gabriel Molina Terriza

- **MEC-MICINN, Adquisición de Equipamiento Científico-Técnico 2018, EQC2018-005100-P**
  XPS microfoco y monocromático para estación ARPES/STM
  PI: Celia Rogero Blanco

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

- **COST Action, Chemistry and Molecular Sciences and Technologies (CMST) 2013, CM1306**
  Modern Tools for Spectroscopy on Advanced Materials: a European Modelling Platform
  PI: Ángel Rubio Secades

- **COST Action, Materials, Physics and Nanosciences (MPNS) 2014, MP1403**
  Nanoscale Quantum Optics
  PI: Javier Aizpurua Iriazabal

- **COST Action, Materials, Physics and Nanosciences (MPNS) 2014, MP1401**
  Advanced fiber laser and coherent source as tools for society, manufacturing and life science
  PI: Joaquín Fernández Rodríguez
  Co-PI: Rolindes Balda de la Cruz

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

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

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

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

- **Marie Curie Individual 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: Ángel Rubio Secades

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

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

- **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: Ángel Rubio Secades

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

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

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

- **FET-OPEN – Novel ideas for radically new technologies (H2020 FETOPEN 01-2016-2017), GA 766864**
  MEMO-Mechanics with Molecules
  PI: Nicolás Lorente Palacios

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

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

- **INTERREG (ETC) V A, cross-border cooperation, POCTEFA (Spain-France-Andorra) 2014-2020, EFA194/16/TNSI**

  TNSI-Trans-Pyrenean Node for Scientific Instrumentation
  PI: Celia Rogero Blanco

- **INTERREG (ETC) VC, interregional cooperation, Aquitania-Euskadi-Navarre Euroregion projects 2017**

  DINaMO-FiVe – 'Durabilidad de Infraestructuras en ambiente marino: NANO-Materiales Optimizados como Fibras Verdes'
  PI: Silvina Cerveny Murcia

- **"Setting up European or International Scientific Networks" (Montage de réseaux scientifiques européens ou internationaux, MRSEI) instrument, ANR-18-MRS1-0014**

  NaWaGui - Nanostructured Waveguides for Photonics
  PI: Rolindes Balda de la Cruz

- **FET-OPEN – Novel ideas for radically new technologies (H2020 FETOPEN 01-2016-2017), GA800923**

  SUPERTED - Thermoelectric detector based on superconductor-ferromagnet heterostructures
  PI: F. Sebastián Bergeret Sbarbaro
  Co-PI: Celia Rogero Blanco

- **NMBP - Nanotechnologies, Advanced Materials, Biotechnology, and Advanced Manufacturing and Processing, Innovative solutions for the conservation of 20th century cultural heritage (H2020-NMBP-35-2017), GA 760858**

  InnovaConcrete - Innovative materials and techniques for the conservation of 20th century concrete-based cultural heritage
  PI: Jorge Sánchez Dolado

- **Marie Curie Individual Fellowship (H2020-MSCA-IF-2017), GA 797109**

  MagicFACE - Magnetic Hybrid Metal-Organic Interfaces
  Supervisor: Enrique Ortega Conejero

- **COST Action, CA17139**

  EUTOPIA - European Topology Interdisciplinary Action
  PI: Ángel Moreno Segurado

TRANSFER OF KNOWLEDGE

In spite of being a fundamental research center, 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 Centers and CICs.

The portfolio of contracts and collaboration agreements with different companies or external parties has been very productive during 2018. Some examples of the partners involved are:

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 (Slovakia)
'Study of hydrated cement pastes'

Francisco José de Caldas University (Colombia)
'Joint actions in the field of materials physics research'

Mujeres por África Foundation
'ELLAS INVESTIGAN project (IV edition). Objective: to promote the leadership of African women in scientific research and technology transfer'

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 above).

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, 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. An example of such initiatives is the starp-up **BihurCrystal**, which is dedicated to the design of ultra-high vacuum (UHV) technologies and new materials for scientific research.

BihurCrystal
www.bihurcrystal.com

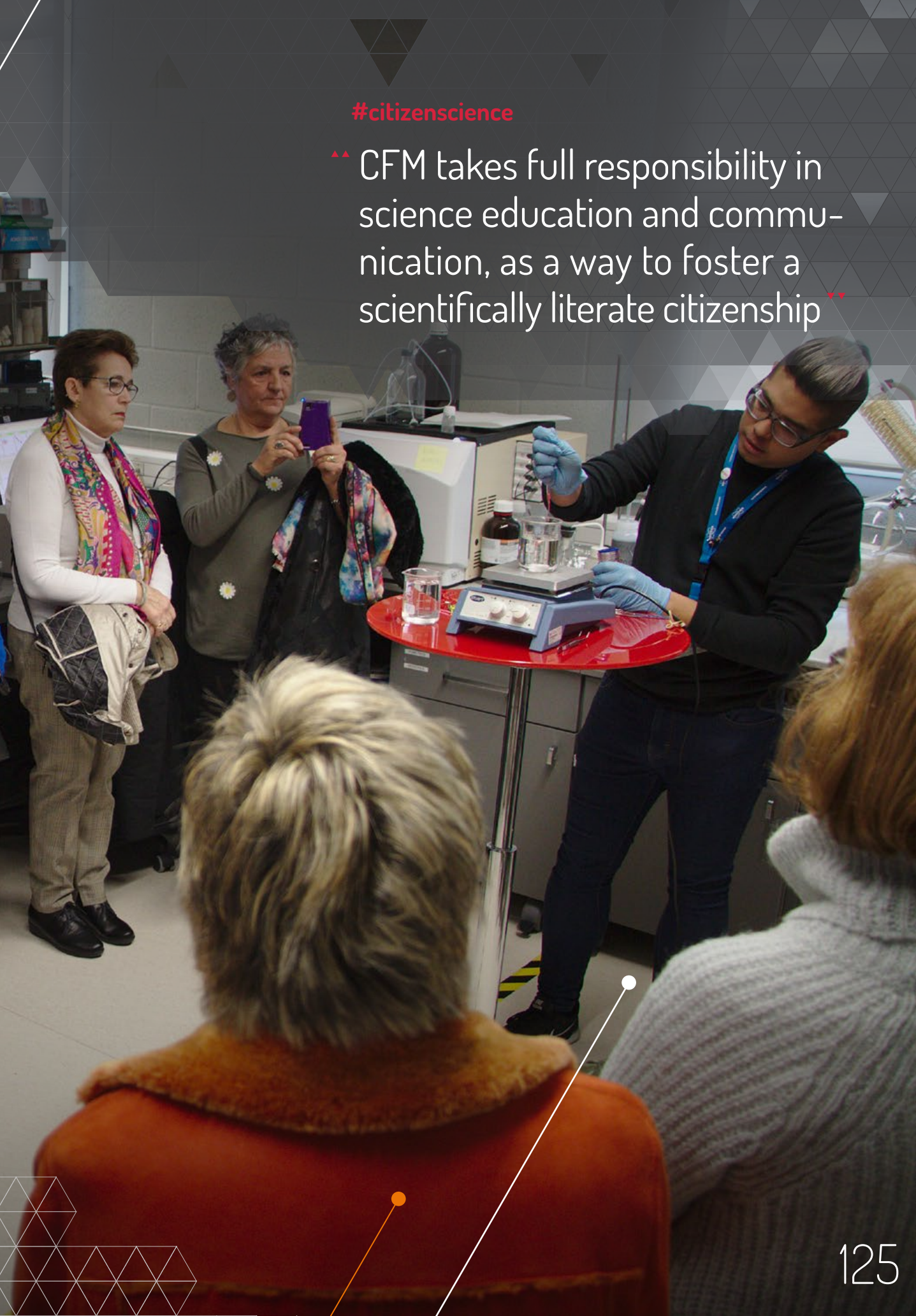
SCIENCE AND SOCIETY

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 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, to PhD students and science communicators.

The efforts at CFM have been devoted to achieve mainly two objectives: spreading scientific culture and generating scientific vocation. Within this spirit, a complete set of scientific outreach activities has been implemented at CFM during 2018.

#citizenscience

"CFM takes full responsibility in science education and communication, as a way to foster a scientifically literate citizenship"



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 centers open their doors to high schools students, approximately every two weeks during the academic year. Besides visiting our facilities, CFM and DIPC offer to 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 2018, CFM had the pleasure to host a total of 15 visits, receiving 499 students, with more than 25 top-line researchers involved in this activity. The calendar of visits during 2018 is displayed below:

JANUARY	FEBRUARY	MARCH	APRIL
Larramendi Ikastetxea (Donostia/San Sebastián)	**Koldo Mitxelena BHI** (Errenteria)	**San Benito Ikastola** (Lazkao)	**Iraurgi Ikastetxea** (Azpeitia)
Colegio Sant Andreu (Barcelona)	**Lekaroz BHI** (Lekaroz, Baztan)	**Urretxu-Zumarraga Ikastola** (Urretxu-Zumarraga)	**Philosophy Faculty** (Donostia/San Sebastián)
Zubiri Manteo BHI (Donostia/San Sebastián)			
MAY	**OCTOBER**	**NOVEMBER**	**DECEMBER**
Aita Larramendi Ikastola (Andoain)	**La Anunciata Ikastetxea** (Donostia/San Sebastián)	**Laskorain Ikastola** (Tolosa)	**Koldo Mitxelena BHI** (Errenteria)
	Saturnino de la Peña (Sestao)	**Usandizaga-Peñaflorida BHI** (Donostia/San Sebastián)	

LANALDI AND MORE

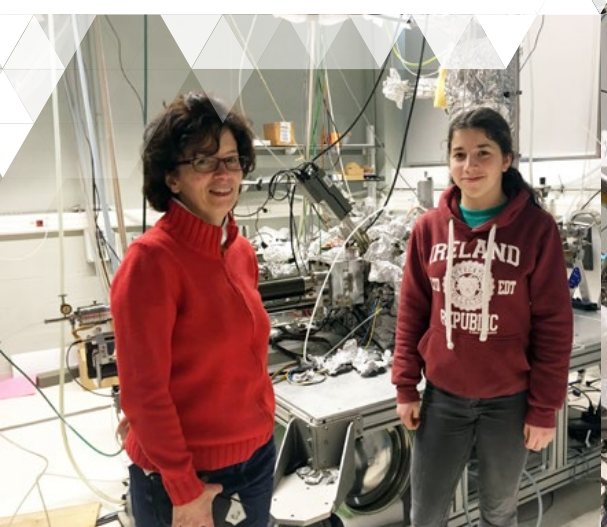
Lanaldi program, organized by "Fundación Novia Salcedo", provides to students a unique opportunity to interact with professionals and share a full day at a scientific center with them in their working places. This is a great chance for young potential researchers to get a real perspective of the daily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

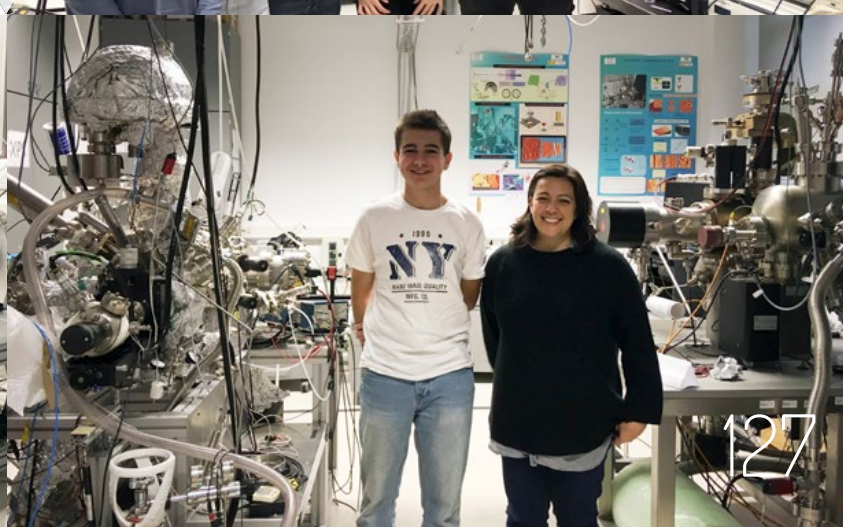
Following the *Lanaldi* program, during 2018 Alba Hernandez Costoya from *IES Solokoetxe BHI* of Bilbao joined the "Spectroscopy at Atomic Scale" group at CFM and shared a day with Lucia Vitali, Ikerbasque Professor and group leader at CFM.

Moreover, at CFM we also try to take care of the requests from individual high school students, who expressed a specific interest to know the center and/or the researchers.

In 2018, Celia Rogero, a tenured scientist from the "Nanophysics Lab" group at CFM and Miguel Moreno, DIPC collaborator at CFM, received the visit of Aritz Izagirre Pardo, from *Asti Leku Ikastola,* whose interests deal with 2D materials and their physical properties.

Daniel E. Martínez Tong, a post-doctoral researcher at the "Polymers and Soft Matter" group, was interviewed by students from St. Patrick's School as part of the program *"El País de los Estudiantes"* yearly organized by the popular national newspaper *El País*.





XVI SCIENCE WEEK (UPV/EHU)

TABAKALERA, DONOSTIA / SAN SEBASTIÁN
8-10 November 2018

Inside the Materials World Stand

From the 8th to the 10th of November of 2018, CFM together with DIPC and CIC nanoGUNE, joined the UPV/EHU's week of science with the stand "Inside the Materials World "at *Tabakalera* cultural center in Donostia / San Sebastián.

Master and PhD students, as well as post-doctoral and permanent researchers of the three centers, got involved in experiments and presentations to show the basis and applications of materials science and some counter-intuitive phenomena to school groups and the general public.

Zientzia Club

10/11/2018

Humor and a lot of science were the components of the *Zientzia Club* formula. At this show organized by UPV/EHU, monologues, talks, performances, or the perfect mix of it all were welcome. In 2018 three members of CFM were premiering on stage. These were the presentations:

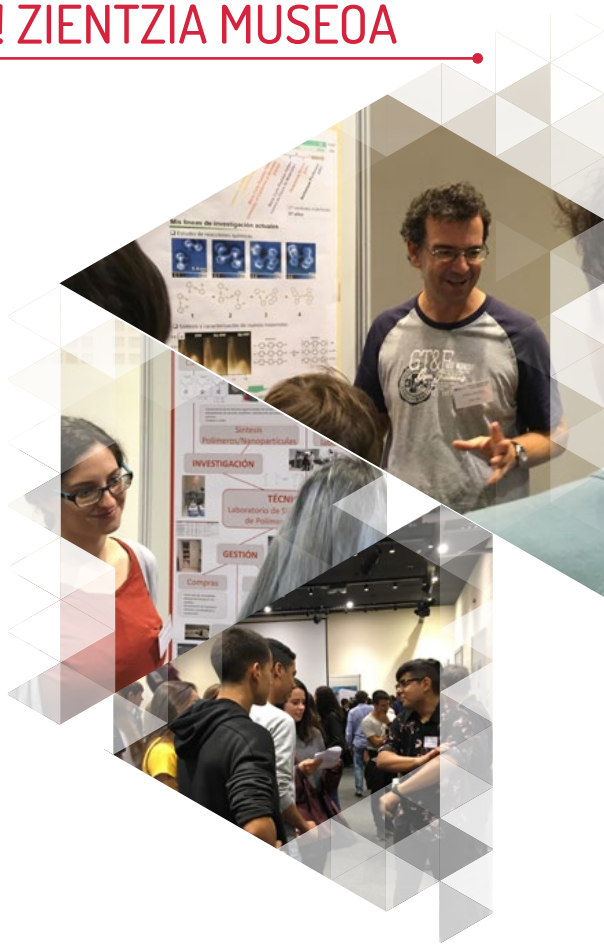
Retorcer la luz, hacer flotar objetos y lo que no te cuentan en el colegio que puedes hacer con la Física
Gabriel Molina

Intolerancia a la viscoelasticidad
Daniel E. Martinez-Tong

Oh my mol!
Idoia Mugica

"A LIFE IN SCIENCE" IN EUREKA! ZIENTZIA MUSEOA

22 October and 5 November



Since 2010, *Eureka! Zientzia Museoa* (the science museum in Donostia / San Sebastián) organizes 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 center who share their experiences.

More than 300 students and 50 professionals attend the meeting yearly.

In 2018, the following researchers from CFM joined this activity:

- **Mª Isabel Asenjo**
  Talk: El orden de los factores no altera el producto

- **Dimas G. de Oteyza**
  Talk and Poster: Física y química de superficies

- **Martina Corso**
  Talk: Materiales ultra-finos para dispositivos electrónicos inteligentes

- **Daniel E. Martinez-Tong**
  Talk: Crecer en un laboratorio y seguir allí 32 años después
  Poster: Microscopia AFM y polímeros

- **Daniel J. Arismendi**
  Poster: Simulando el comportamiento de una substancia aparentemente ordinaria, sin embargo realmente misteriosa: El agua

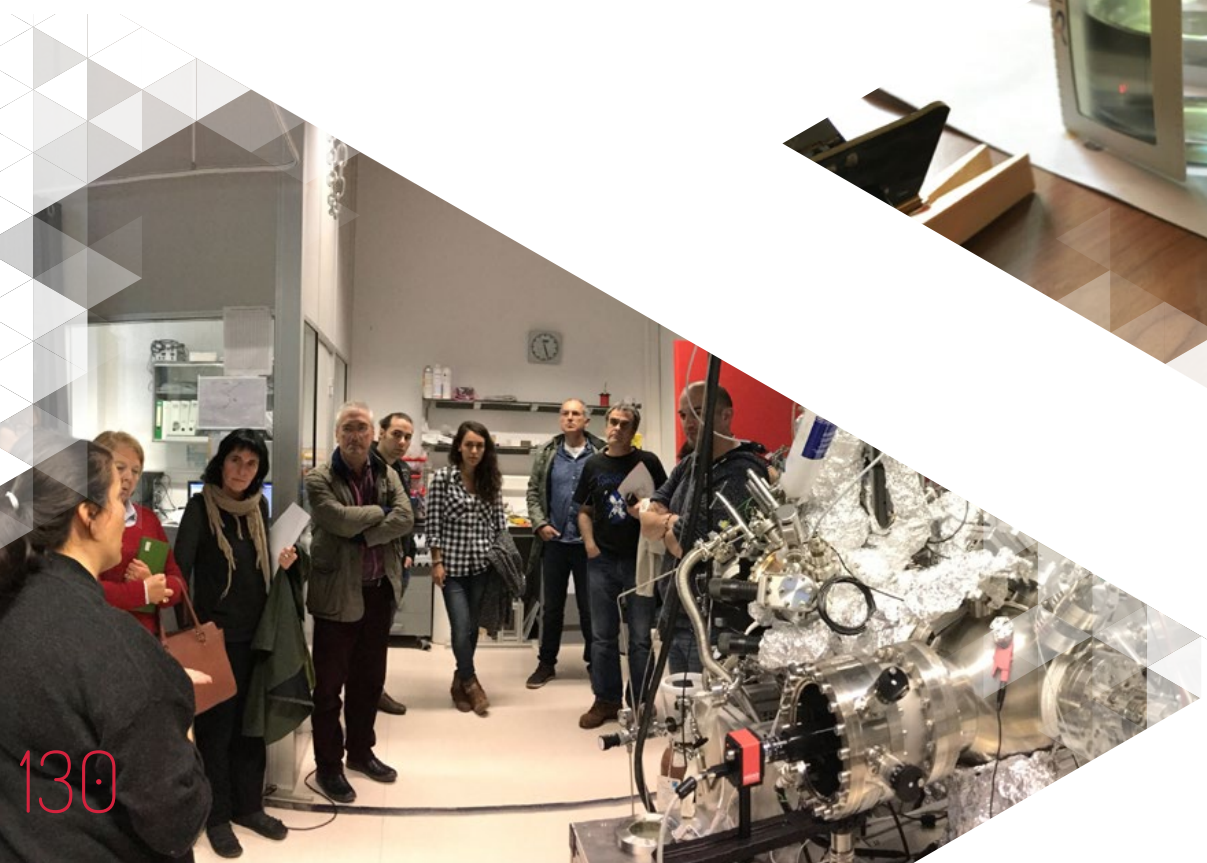
- **Julen Ibañez**
  Poster: Munduko pilota partidarik txikiena

LIGHT WORKSHOP

CFM
10 May 2018

The 39th session of UNESCO's General Conference proclaimed 16 May as "International Day of Light". On the occasion of this event, Gaizka Durana and Gotzon Aldabaldetreku from the Applied Photonics Group of the UPV/EHU, in collaboration with the Science Advisory team of the Basque Government *(Berritzegune Nagusia),* and CFM organized this course-workshop, aiming at secondary school teachers. The idea was to provide practical activities to be ran at the classroom, highlighting the central role played by technologies based on light and the power of light in the lives of world citizens in the areas of science, technology, culture, education and sustainable development.

25 teachers participated in this hands-on workshop that included an introductory talk on the field by Javier Aizpurua, director of CFM and head of the "Theory of Nanophotonics" group at CFM, and a visit to the "Nanophysics Laboratory" of CFM.



"QUÉ SABEMOS DE..." TALK SERIES

TABAKALERA, DONOSTIA / SAN SEBASTIÁN
9, 16, 23 and 30 November 2018

Qué sabemos de... is a peculiar series of outreach talks inspired by the intrinsic curiosity of the human being. The program included hot topic and renowned speakers, and was organized by CFM and CSIC, at the iconic cultural center *Tabakalera* in Donostia / San Sebastián, with the collaboration of *Kutxakultur*.

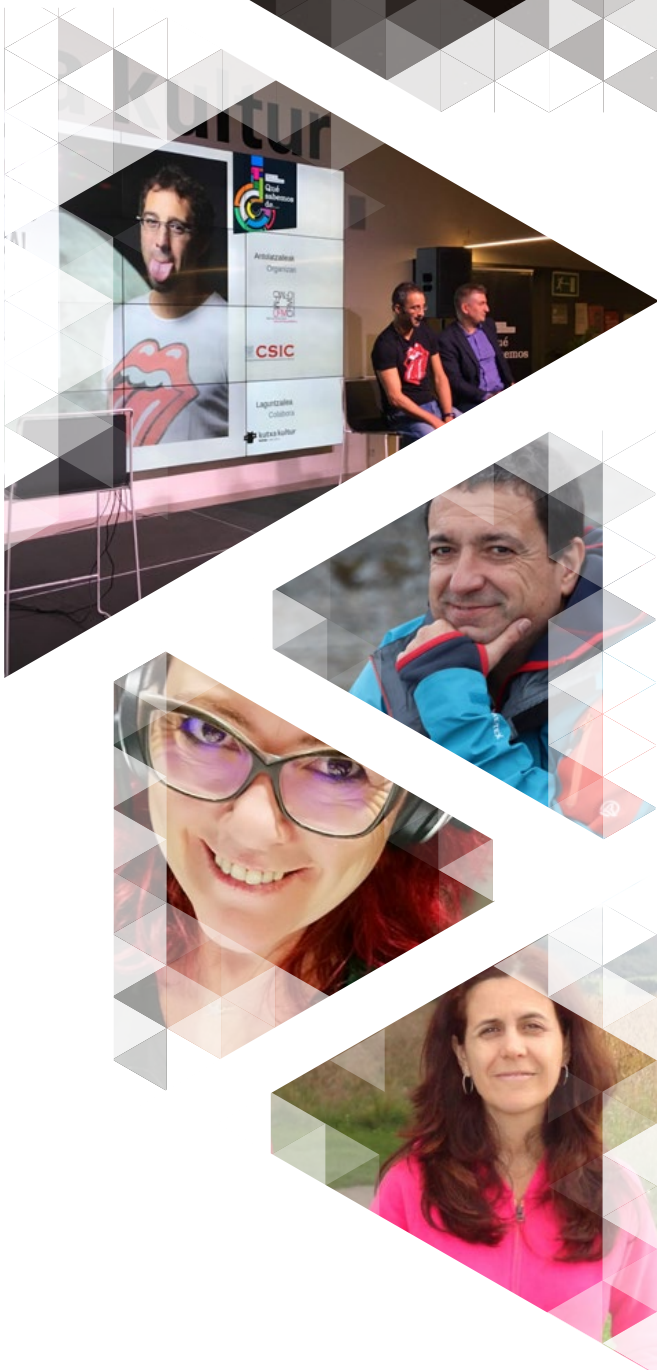
More than 500 attendees participated in the 4 talks organized in this edition of the talk series. These were the talks of 2018:

La Antártida como centinela de la contaminación global
Jordi Dachs

Exoplanetas, astronomía y...¡Música!
Jose A. Caballero

Escutoides, una historia de matemáticas bajo nuestra piel
Clara Grima

Del electrón al chip
Gloria Huertas



Available at CFM's YouTube channel or scanning this code

PINT OF SCIENCE

pintofscience.com
14-16 May, 2018

The "Pint of Science" festival aims to deliver interesting and relevant talks on the latest science research in an accessible format to the public – mainly across bars and pubs. The goal is to provide a platform, which allows people to discuss research with the people who carry it in a friendly environment, such as a pub. Run mainly by volunteers, in 2018, CFM supported this festival that filled up our city with science. Cheers!!!

In addition, Celia Rogero, a tenured scientist from the "Nanophysics Laboratory" group at CFM, participated in the festival with the following talk:

La vida secreta de las moléculas
Celia Rogero
14/05/2018

PARTICIPATION IN OUTREACH TALKS

Naukas Donostia
Victoria Eugenia Theatre
19/05/2018

Organized by Naukas and DIPC, CFM collaborated in the edition of Naukas Donostia in 2018. In this edition, three members of the CFM, among many other amazing speakers, came out to the stage of a theatre that hung the sold out poster:

Papiroflexia a la 10-9
Sara Barja

Ver o no ver, esa es la cuestión
Javier Aizpurua

De lo pequeño a lo grande
Pedro Miguel Echenique

Available at Kosmos (EITB) or scanning these codes

Azaroa, zientziaroa

9/11/2018

Within the activities of outreach developed by the Lemniskata organisation in the Goierri area of the province of Gipuzkoa, a special set of talks on Science was held in November 2018. The following outreach talk was given in Beasain:

Argia txikia egiten denean (When light goes small, in Basque)

Javier Aizpurua

15TH EDITION OF PHOTO EXHIBITION "FOTCIENCIA"

CRISTINA ENEA FOUNDATION

3-30 September 2018

FOTCIENCIA is a Photography contest organized yearly by *Consejo Superior de Investigaciones Científicas* (CSIC) and *Fundación Española para la Ciencia y la Tecnología* (FECYT) in collaboration with *Jesús Serra* foundation. The aim of the initiative is to bring science closer to the society inviting researchers as well as citizens to participate in two categories: macro and microscopic photography. As a result of the contest, a photo exhibit is yearly launched. This exhibit travelled more than 20 cities in 2018, and CFM had the pleasure to bring it to Donostia / San Sebastian, continuing with the tradition implemented during the last three years.

In 2018 the exhibition was opened to the public from the 3rd to the 30th of September at the environmental resource center of the *Cristina Enea* Foundation, thanks to the agreement signed with this foundation.

BRICOMICRO: SCALE YOUR WORLD

CRISTINA ENEA FOUNDATION
29 September 2018

This workshop aimed explorers between 4 and 12 years old. How far do our eyes see? With this moto, 25 kids and their families, guided by CFM researchers and experts in the field, discovered the world of macro, micro and nanoscopic scales, by collecting samples in the park of *Cristina Enea* and putting them under a home-made microscope and different magnifying glasses.

INTERNATIONAL WOMEN AND GIRL IN SCIENCE DAY 2018

Materialen Fisika Zentroa
Centro de Física de Materiales
Materials Physics Center

Donostia International Physics Center

CIC nanoGUNE
nanoscience cooperative research center

CIC biomaGUNE
Biomaterialetako Ikerkuntza Kooperatiboko Zentroa
Centro de Investigación Cooperativa en Biomateriales

SCIENCE IS INDEED A GIRL THING

In order to achieve access and full and equal participation in science for women and girls, in 2016 the United Nations General Assembly decided to proclaim 11 February as International Women's and Girls' Day in Science.

On February 8 and 9, 2018, CFM, CIC nanoGUNE, CIC biomaGUNE and DIPC commemorated this day, and joined forces to make visible the activity of women in science, and to break with the typically masculine roles attributed to scientific-technical activities and encourage the choice of scientific careers among girls and adolescents.

In an unprecedented collaboration, with more than 40 volunteers on board, the 4 centers joined forces to present a full program that aimed women teenagers, school kids, elder women (above 55), citizens in general and the scientific community.

INTERNATIONAL WOMEN AND GIRL IN SCIENCE DAY 2018

1. Do you know any women in science?

February 8
Public: School children
Venue: CIC nanoGUNE

In 2018, around 50 students from Ibai Ikastola and San Alberto Magno Deutsche Schule participated in this workshop, led by women researchers of CIC nanoGUNE.

2. Donostia: City of women researchers

(Available at CFM's YouTube channel)
February 8
Public: Open
Venue: Koldo Mitxelena, Donostia / San Sebastián

Short outreach talk session were also given by women researchers from the organizing centers:

- **¿Cómo se ven las cosas muy pequeñas?**
  Sara Barja Martínez (Ikerbasque Research Fellow at CFM and associated researcher at DIPC)

- **Historia de la ciencia de materiales: de la edad de piedra a la clasificación topológica**
  Maia García Vergniory (Ikerbasque Research Fellow, DIPC. Loreal Women Researcher Award 2017)

- **Mundo Superconductor**
  Deung-Jang Choi (Ikerbasque Research Fellow at CFM. Guest Researcher at CIC nanoGUNE)

- **Cuando la luz encuentra la materia en la nanoescala**
  Marta Autore (Post-doctoral Researcher at CIC nanoGUNE)

- **Diseño de proteínas para construir LEGOs moleculares**
  Aitziber López Cortajarena (Ikerbasque Research Professor at CIC biomaGUNE)

Available at CFM's YouTube channel or scanning this code

3. Amona's power

February 9
Venue: CFM
Public: + 55 year old women

The aim of this workshop was to find the scientific potential hidden behind everyday things, allowing the scientist that lives inside anyone to get out, and empowering women to be the ultimate science ambassadors. 35 women joined the visit and shared this unique experience with all the volunteers.

INTERNATIONAL WOMEN AND GIRL IN SCIENCE DAY 2018

4. Science is indeed a girls' thing.

February 9
Venue: CIC nanoGUNE
Public: Teenager women

Led by the female researchers of the centers, more than 30 teenagers had the opportunity to be "scientists for a day" and perform hands-on experiments in nanoscience.

5. High-school visit

February 9
Venue: DIPC and CFM
Public: Teenagers
Exclusively women-driven visit for teenagers.

6. WinS Colloquium: Career development outside academia

February 9
Venue: CIC biomaGUNE
Public: Scientific Community

In this seminar, Dr. Alba Centeno Perez *(Graphenea)* & Dr. Africa G. Barrientos *(Midatech Pharma)* gave their view on switching career from academia to industry, prospects, and outcomes. After short talks, an open discussion brought the opportunity to young and senior researchers to discuss with them the pros and cons of a career development outside academia in local companies.

EUSKAL ESPERIENTZIAK ZIENTZIA ZABALKUNTZAN (EEZZ18)

eezz18.dipc.org
14-15 June, 2018

CFM, together with the Chair of Scientific Culture of the UPV/EHU and DIPC, organized this congress in which more than 80 professionals from the field of communication and scientific dissemination of the Basque Country came together to share experiences and good practices. With practically all the agents represented, the main objective proposed and achieved was to compose the general map of the initiatives carried out for the communication and dissemination of science in the Basque Country and to consolidate a forum among the agents gathered.

ACTIVITY IN MASS MEDIA

During 2018, CFM was cited over 148 times in the media, including press, online articles, TV and Radio.

Press articles
47*

Online press
80*

Radio
19

TV
2

*Scientific publications excluded

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.

COLLABORATION NETWORK

CFM 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

CIC biomaGUNE

Cristina Enea Fundazioa

Diputación de Guipuzkoa- Gipuzkoako Foru aldundia

Aulas Kutxa- kutxakultur

Eureka! Zientzia museoa

Norteko Ferrokarrila

La Mecánica del Caracol

Cátedra de Cultura Científica (UPV/EHU)

Pint of Science

FECYT

Fundación Novia Salcedo

Berritzegune Nagusia

Asociación Española de Comunicación Científica

MISCELLA-NEOUS

FROM DELAWARE TO DONOSTIA / SAN SEBASTIÁN UNITING SCIENCE AND CULTURE

During the month of January 2018, CFM hosted the visit of 20 students from the University of Delaware, in the United States. In this unprecedented collaboration an innovative transdisciplinary course *"a la carte"* was designed, in which material physics classes and a specialized course in the history of the Basque Country were combined.

This course was a unique opportunity to intertwine two seemingly distant disciplines in an effort to foster a global and transdisciplinary culture that does not distinguish *"sciences"* from *"humanities"*.

PHD RECRUITMENT FAIR 2018

In 2018 CFM organized a PhD Recruitment Fair as part of the strategic plan to recruit new talent. From the applications received, 25 candidates were shortlisted by a selection committee of the center and invited for a 2-days visit to CFM, with their travel and accommodation expenses fully covered. Personal interviews were held and the candidates had the opportunity to discuss the research projects with CFM researchers.

After the evaluation, 8 candidates were selected and granted full studentships to join one research group at CFM:

- **Marina Peña Díaz**
  (Nanophysics Lab)
- **Carmen González Orellana**
  (Nanophysics Lab)
- **Cristina Mier González**
  (Quantum Phenomena on Surfaces)
- **Joseba Goikoetxea Perez**
  (Modelisation and Simulation)
- **Miguel Ángel Jiménez Herrera**
  (Souza Research Group)
- **Jon Lasa Alonso**
  (Quantum Nanophotonics Lab)
- **Mariarita Paciolla**
  (Polymers and Soft Matter)
- **Óscar Rodríguez Ballesteros**
  (Materials Computation and Theory)

CFM AND WOMEN FOR AFRICA

GIPUZKOA COOPERA program with the Women for Africa Foundation, DIPC, ASPEGI and CFM

Gipuzkoa Coopera is a project launched by the Provincial Council of Gipuzkoa in 2017 and aims to promote Development and Cooperation by extending them to non-conventional activities.

In 2018, two main activities were launched within this scheme of collaboration: *Ellas investigan* and *Baratzatik merkatura,* the first one to be carried out by at the CFM and DIPC research centers, and the latter, accomplished by the association of Professionals and Businesswomen of Gipuzkoa, ASPEGI, in close collaboration with the Foundation Women for Africa.

Thanks to this initiative, two African researchers will carry out six-month research stays at DIPC and CFM during 2019, and five Tanzanian entrepreneurs, under the auspices of ASPEGI, arrived to Donostia / San Sebastián in 2018 to learn about different agro-food experiences in order to develop and improve their business projects. Each of these actions was financed by the Provincial Council of Gipuzkoa with 25.000 euros.

The female African researcher visiting and collaborating at CFM is Dr. Njukeng Jetro Nkengafac from Cameroon who collaborates with Prof. Ángel Alegría in the Polymers and Soft Matter group at CFM.

CFM makes the words of the Deputy for Culture and Cooperation of Gipuzkoa our own:

"We are giving a strategic turn to cooperation policies looking towards Africa and with these women who come to Gipuzkoa all stereotypes are broken. These researchers and entrepreneurs are coming to broaden and share their knowledge, and then pass it on."

LEARN AFRICA

Together with the *Ellas investigan* program, the Women for Africa Foundation launches "Learn Africa", an initiative that aims to promote the transfer of knowledge, exchange and training of undergraduate and graduate African women students through scholarships in Spanish universities that collaborate in this initiative.

In 2018, DIPC and CFM joined the program and offered a grant that fully covers the stay and expenses of a student to enroll in the Master in Nanoscience of the UPV/EHU. The recipient of the scholarship was Afia Owusuah Akyaw from Ghana, who develops her master thesis at CFM under the supervision of Sara Barja and Celia Rogero at the Nanophysics Lab.

OPENING OF THE QUANTUM NANOPHOTONICS LAB

In 2018 the Quantum Nanophotonics Lab, led by Ikerbasque Research Professor Gabriel Molina-Terriza, was launched at CFM. This is a strategic asset for the CFM research lines, as it aligns the centre with the international context on the experimental development of Quantum Technologies. The Quantum Nanophotonics Lab will be mainly dedicated on developing new measuring techniques and sensing devices at the very limit of precision and sensitivities allowed by Nature. In particular, they will develop new quantum sources of light capable of observing properties of nanoparticles which are hidden in conventional microscopes. On the other hand, our team of researchers will exploit the quantum properties of nanoparticles in order to forge a new set of quantum enhanced magnetic, inertial and molecular sensors.

HIGHLY CITED RESEARCHER 2018

PROF. JAVIER AIZPURUA IRIAZABAL

After being included for the first time in 2017, Professor Javier Aizpurua remains in the 2018-list of the most cited researchers in the world, according to the database drawn up by Clarivate Analytics. Prof. Javier Aizpurua, head of the "Theory of Nanophotonics" group at CFM and DIPC, and director of CFM, has been recognized as a highly cited researcher in 2018, for the second consecutive year, based on the highly cited papers from 2006 to 2016.

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. Javier Aizpurua is one of the 5 highlighted researchers in the area of Physics developing their work in Spain.

According to the impact of the list in the Basque Country, and considering all the science fields, four other researchers received a similar recognition in the Basque Country: Ángel Borja (AZTI), Luis M. Liz-Marzán (CIC biomaGUNE), Maurizio Prato (CIC biomaGUNE) and Wolfgang Parak (CIC biomaGUNE).

THE ELEMENTS OF CFM

cfm.ehu.es

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