CFM

Materialen Fisika Zentroa

Centro de Física de Materiales

Materials Physics Center

ACTIVITY REPORT

2019

CSIC
Consejo Superior de Investigaciones Científicas

eman ta zabal zazu
Universidad del País Vasco
Euskal Herriko Unibertsitatea

MPC-BERC
Materials Physics Center
Basic Excellence Research Centre

ACTIVITY REPORT 2019

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SUMMARY

FOREWORD

> The secret of our success is, undoubtedly, having the support and closeness of a team of such human quality and professionalism in our daily activities as that of CFM

Andrés Arnau Pino, Vicedirector

We are writing these lines at the beginning of May 2020. These are dark times, the ***Centro de Física de Materiales*** (CFM) has been closed, without any on-site activity, since March 16 as a consequence of the measures taken to fight the Covid-19 pandemic that is causing so much uncertainty and grief worldwide. CFM staff is demonstrating a commendable degree of commitment, thanks to which many of the programmed activities continue in spite of these exceptional circumstances. It is in these difficult times, in which most of us have been confined in our homes for almost two months and in which we miss the contact with friends and loved ones, that we appreciate more clearly than ever the importance of having the support and closeness of a team of such human quality and professionalism in our daily activities as that of CFM. This is undoubtedly the secret of our success: A group of fully committed and enthusiastic professionals that manage to create the most favorable atmosphere for every member of the community to achieve its top performance.

The year 2019 was a clear demonstration of this excellence. It was certainly a good year for CFM in terms of scientific production. More than 190 indexed publications (including some in the highest impact journals), 70 ongoing research projects (20 of them European and international ones, including one ERC starting grant), with more than 4.8 million € granted to CFM researchers only in 2019, 8 PhD theses defended, and one of our scientist, Prof. Eugene Tchoulkov, received the Euskadi Research Prize 2018, congratulations Eugene!

In addition, many scientific events, such as seminars, workshops, conferences and outreach activities have taken place at CFM. Every single contribution matters, and we all are part of this success. We are proud to decisively contribute to put in the map Basque research in the area of Materials Science.

During 2019 the CFM family grew with new permanent researchers. On the one hand, Professor Ikerbasque Félix Fernández Alonso joined CFM to promote the use of neutron techniques in the characterization of materials beyond polymer science, the latter a traditional and powerful research line at CFM. On the other hand, three researchers obtained permanent positions from CSIC to join CFM: Marek Grzelczak, who will incorporate new expertise to CFM related to the synthesis and characterization of nanomaterials

Daniel Sánchez Portal, Director

> The level of international recognition that we have achieved is only possible thanks to the commitment of all CFM personnel and to the decisive and continuous support of the institutions behind CFM

for health care and energy applications; Pedro Braña Coto, who will join the already powerful line of ab initio simulations, with a twist towards molecular physics in relation with optoelectronics and energy applications; and Ruben Esteban, who will reinforce the line of theory of nanophotonics and nanoplasmonics.

Summer of 2019 was marked by two events that filled the CFM community with sadness. Two dear companions left us forever. Juanjo del Val Altuna passed away in July. He was a researcher and a professor at the Department of Materials Physics at UPV/EHU. He had been a member of the CFM since its creation in 1999 and had only retired a few months earlier. A few days later, we received another shocking blow, the loss of one of the most recent additions to the CFM family, Alberto Sainz de Murieta Alvarez, who had assumed the duties of Administration Manager just a year earlier. Despite the short time he had been with us, Alberto had decisively taken the reins of the CFM administration and had earned a place in the hearts of all of us with his calm style, good manners and know-how. We miss these two dear friends.

Autumn 2019 began with a change in the direction of CFM, which was assumed by Daniel Sánchez Portal. Javier Aizpurua Iriazabal left after four very productive years in office. Andrés Arnau Pino continued in his position as CFM Deputy Director and assumed the position of Acting Administration Manager. We thank Javier for his great effort and dedication, which is reflected in the excellent trajectory and the good atmosphere of the center during the last years.

Achieving international recognition in basic research is not an easy task. We have to compete with laboratories developing cutting-edge science all over the world. Succeeding in this challenge is only possible thanks to the commitment of all CFM personnel and to the decisive and continuous support of the three key institutions behind CFM, CSIC, UPV/EHU and the Basque Government. We also count on the support from Gipuzkoa Province Government via competitive calls to promote strategic activities. With these four allies, we are fully confident that we will continue the brilliant upward trajectory of CFM in the next years. Thank you all for your commitment and support.

Daniel Sánchez Portal
Andrés Arnau Pino

In memorian of Alberto Saínz de Murieta

Este año hemos sufrido la pérdida de Alberto Saínz de Murieta. Alberto se había incorporado recientemente al equipo de dirección del CFM como gerente del mismo, y en poco tiempo se convirtió en una persona muy querida tanto por su calidad humana como profesional. Como director del CFM en aquel tiempo, no podía intuir que, en pocos meses, Alberto sería depositario de toda mi confianza y cómplice fundamental en la toma de decisiones que afectaban al centro. Alrededor nuestro, ese sentimiento de comodidad y confianza en relación a su actividad y a su personalidad se extendía a toda persona que interaccionaba con él, bien fuera gestora, o científica.

Alberto trajo muchas cosas buenas al CFM, entre ellas, seguridad, confianza, mesura, tranquilidad, profesionalidad, respeto, bondad, y buen hacer. Además, Alberto estaba encantado en el centro y así me lo dijo el par de veces que le pregunté explícitamente sobre ello. Yo solo puedo decir que siempre admiraré a Alberto por su dedicación, y su alto nivel de excelencia en todo lo que hacía. Alberto era el complemento administrativo y humano perfecto para la actividad científica del centro, algo que demostró en un tiempo record, sin prisa, pero sin pausa y, por ello, los que le conocimos le estaremos siempre agradecidos.

Nos ha dejado una persona fantástica de manera repentina, ocasionando un vacío enorme en nuestro corazón. Compartimos el dolor con su compañera Mariví, y su hijo Peru, a los que nos unimos en el último adiós del centro a Alberto, y a los que ya siempre nos unirá el cariño. Nos queda la satisfacción de que Alberto viera concluido uno de sus pequeños proyectos en el centro: el diseño, solicitud, y ejecución de un parking de bicis para el personal del centro. Tuvimos ocasión de dedicar a Alberto nuestro parking junto a su familia y amigos, en un acto entrañable de una tarde preciosa de septiembre. El parking de Alberto nos evoca su persona y su acción, que nunca olvidaremos.

El mejor homenaje que le podemos hacer es precisamente recordarle, ahora y siempre, como una de las personas que hizo del CFM un centro mejor, y que nos hizo también mejores a los que le rodeábamos.

(Original words from the author)

This year we have suffered the loss of Alberto Saínz de Murieta. Alberto had recently joined the management team of the CFM as its manager, and in a short time he became a much loved person both for his human and professional qualities. As director of the CFM at that time, I could not have imagined that, in a few months, Alberto would be the depositary of all my trust and a fundamental accomplice in the decisions that affected the center. Around us, that feeling of comfort and trust in relation to his activity and personality extended to everyone who interacted with him, whether he was a manager or a scientist.

Alberto brought many good things to the CFM, among them, security, confidence, moderation, tranquility, professionalism, respect, kindness, and good work. In addition, Alberto was delighted at the center and told me so the couple of times I explicitly asked him about it. I can only say that I will always admire Alberto for his dedication, and his high level of excellence in everything he did. Alberto was the perfect administrative and human complement to the scientific activity of the center, something he demonstrated in record time, without hurry, but without pause, and for this, those of us who knew him will always be grateful to him.

Alberto, a fantastic person, has left us in a sudden way, causing a huge void in our hearts. We share the pain with his companion Mariví, and his son Peru, who we join in the last goodbye of the center to Alberto, and to which we will always be united by love. We are pleased that Alberto saw one of his small projects at the center completed: the design, application, and execution of a bicycle parking lot for the center's staff. We had the opportunity to dedicate our parking lot to Alberto, together with his family and friends, in a lovely act on a beautiful September afternoon. Alberto's parking evokes his person and his action, which we will never forget.

The best tribute we can make to him is precisely to remember him, now and always, as one of the people who made the CFM a better center, and who also made those around him better.

Javier Aizpurua

In memorian of Juanjo del Val Altuna

El día 24 de Julio de 2019 nos dejó para siempre Juan José del Val Altuna víctima de una severa enfermedad que terminó con su vida demasiado rápido. Juanjo era profesor universitario en el Departamento de Física de Materiales de la Universidad del País Vasco desde los años 80 y miembro del Centro de Física de Materiales desde su fundación. Menos conocida es su faceta de gran montañero con un conocimiento exhaustivo de los 500 kilómetros de Pirineo, algo que le gustaba compartir con colegas y amigos.

On July 24, 2019, Juan José del Val Altuna passed away a victim of a severe illness that ended his life too quickly. Juanjo was a university professor in the Department of Materials Physics at the University of the Basque Country since the 1980s and a member of CFM since its foundation. Less well known is his facet as a great mountaineer with an exhaustive knowledge of the 500 kilometres of the Pyrenees, something he liked to share with colleagues and friends.

Juanjo impartió docencia en materias del grado en la Facultad de Química (clases teóricas, problemas, prácticas de laboratorio…) y en posgrado (master de Nanociencia, doctorado…). En investigación científica, son notables sus trabajos y publicaciones sobre materiales poliméricos y metálicos con carácter amorfo (nanocristalino, nanogranular) siendo una autoridad científica en caracterización microestructural por técnica de difracción de rayos X.

Juanjo taught undergraduate subjects in the Faculty of Chemistry (theory classes, problems, laboratory practices...) and postgraduate subjects (master's degree in Nanoscience, doctorate...). In scientific research, his works and publications on polymeric and metallic materials with amorphous character (nanocrystalline, nanogranular) are remarkable. He was a scientific authority in microstructural characterization by X-ray diffraction techniques.

La pérdida de Juanjo ha supuesto un varapalo para todos los que tuvimos la suerte de conocerle. Siempre recordaremos su pasión y entusiasmo impartiendo clases, o en el laboratorio mientras hacía medidas. También recordaremos su carácter noble y apasionado, que plasmaba en largas y vívidas tertulias con los amigos, donde nunca faltaban ni la vehemencia de sus afirmaciones ni su franca sonrisa, la cual ha quedado grabada en nuestra memoria.

The loss of Juanjo has been a shock for all of us who were lucky enough to know him. We will always remember his passion and enthusiasm for teaching, or in the laboratory while making measurements. We will also remember his noble and passionate character, which he captured in long and vivid discussions with friends where neither the vehemence of his statements nor his frank smile, which remains engraved in our memory, were ever missing.

(Original words from the authors)

Iñaki Juaristi and Andres Arnau

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: **Daniel Sánchez Portal**

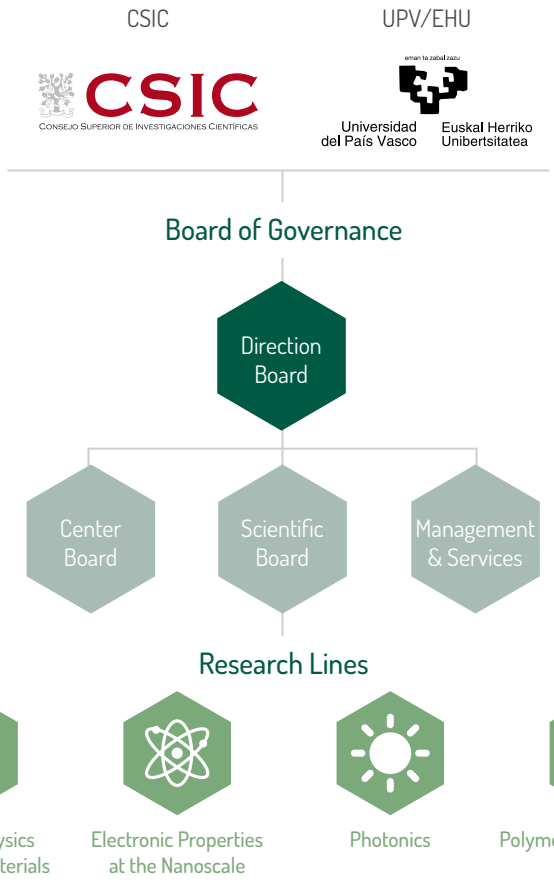
Vice director: **Andrés Arnau Pino**

Secretary: **Amaia González Azpeitia**

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.

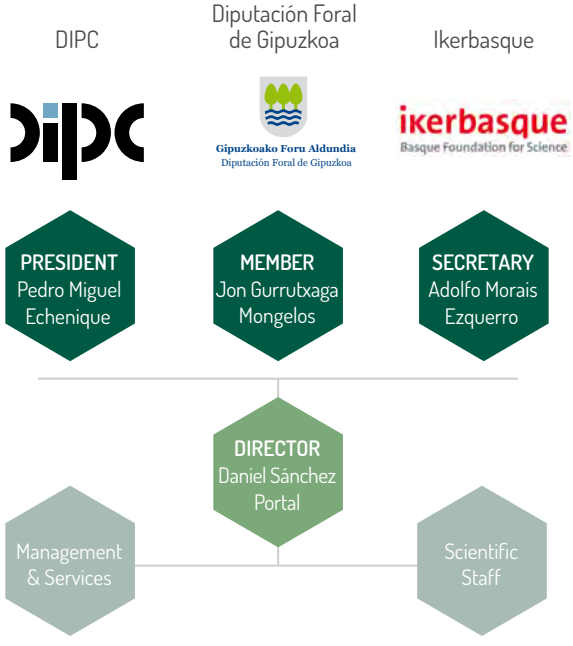
CFM



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 Ikerbasque Foundation, the Gipuzkoa Provincial Council (*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

RESEARCH COMMUNITY

Researchers in Action

224*

♀ 67 ♂ 157

* Including visiting researchers, undergraduate and master students

16

Research Groups

RESEARCH OUTPUT

ISI Publications

199

International Collaborations

79%

H Index

125

Q1 Publications

71%

Citations*

11289

* Source: Publons as of March 2020

ACTIVITIES AND EVENTS

Seminars

20

Conferences, Workshops and Courses

14

Visitors from Schools

549

Outreach Activities

23

54%
of the Research Community is international

Researchers from
36
countries

PROJECTS AND FUNDING

Ongoing Projects
70

Funding
6 041 202 €

TRAINING

8
PhD Theses defended

13
Pre-doctoral Researchers' Stays Abroad

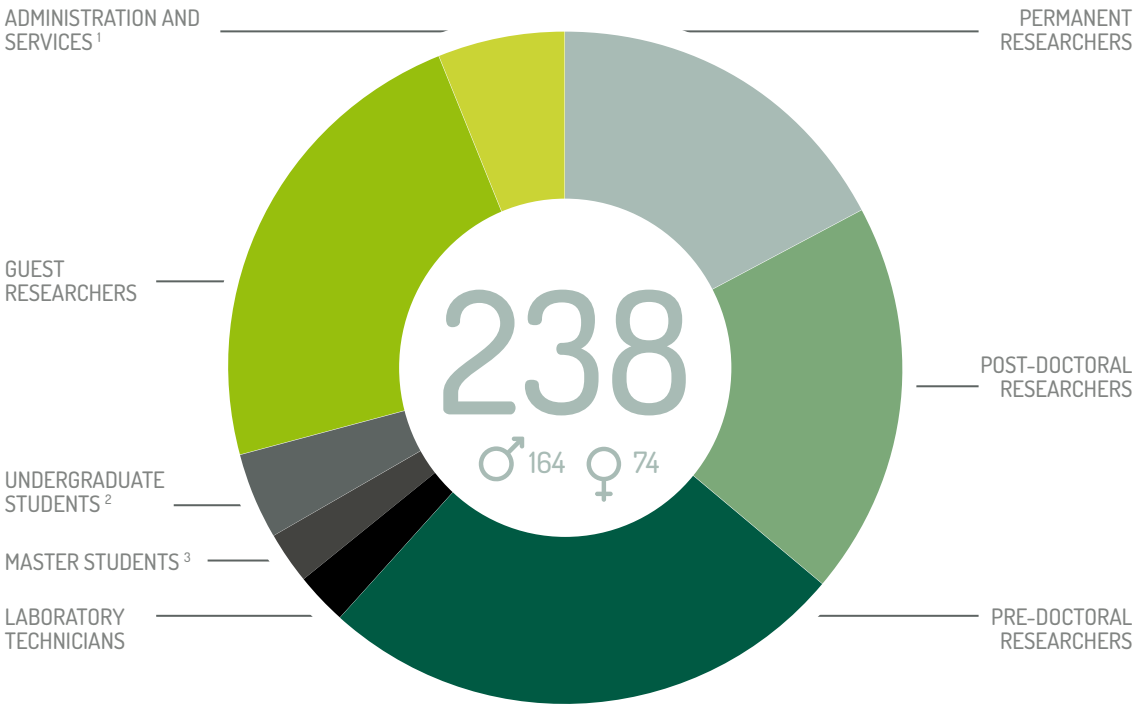
9
Master Theses Defended*

4
Undergraduate Projects Defended

* In the framework of the nanoscience master or supervised by CFM staff

PEOPLE

ALL THE CFM COMMUNITY



CFM Staff

172

Researchers in Action

224 [4]

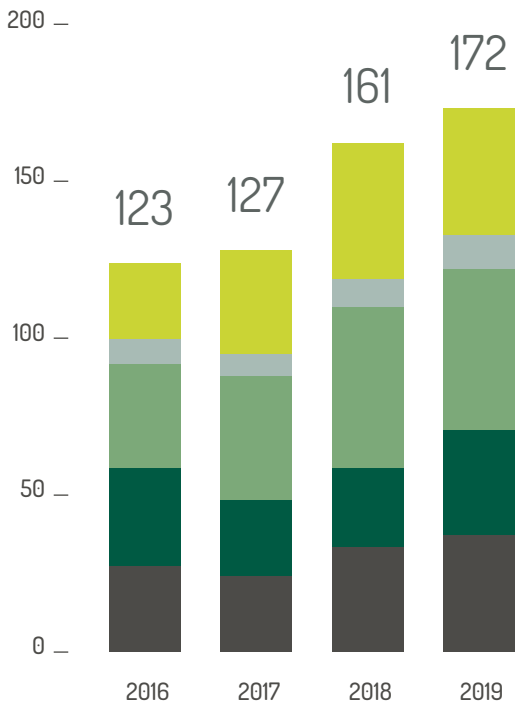
Permanent Researchers	41
Post-doctoral Researchers	45
Pre-doctoral Researchers	61
Laboratory Technicians	6
Master students [3]	6
Undergraduate students [2]	10
Guest Researchers	55
Administration and Services [1]	14
Total	238

[1] One of those did an internship and is not considered staff
[2] Three of those received scholarships during their stay at CFM and are considered staff
[3] Three of those received scholarships during their stay at CFM and are considered staff
[4] Including Guest researchers, undergraduate and master students

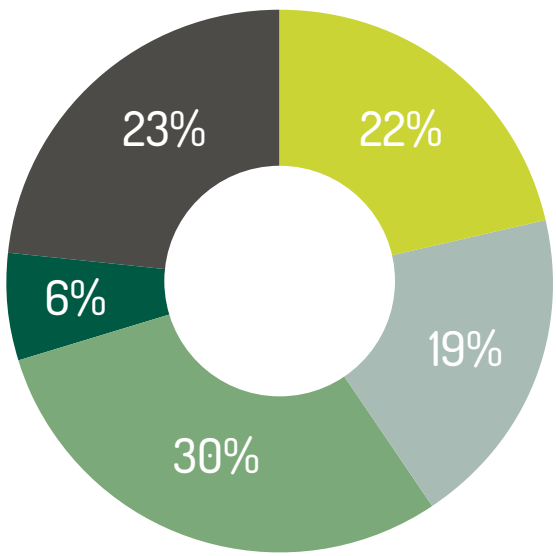
DISTRIBUTION OF CFM STAFF
according to the origin of their financial support

	2016	2017	2018	**2019**
CSIC	27	24	33	**37**
UPV/EHU	31	24	25	**33**
MPC-BERC	33	39	51	**51**
IKERBASQUE	8	7	9	**11**
COLLABORATORS	24	33	43	**40**
Total	123	127	161	**172**

Distribution of CFM staff in absolute numbers according to the origin of their financial support through the years



Distribution of CFM staff in percentage according to the origin of their financial support in 2019



DIRECTION BOARD

Before October 2019

Director: Javier Aizpurua Iriazabal

Vicedirector: Andrés Arnau Pino

General Manager: Alberto Saínz de Murieta Álvarez (in memoriam)

From October 2019

Director: Daniel Sánchez Portal

Vicedirector: Andrés Arnau Pino

General Manager: Amaia González Azpeitia (incorporated in April 2020)

ADMINISTRATION AND SERVICES

Administration

Adolfo del Arco García, **Administrative,** CSIC

Alberto Saínz de Murieta Álvarez (in memoriam), **Administration Manager,** CSIC

Ane Iturriza Semperena, **Administrative,** MPC

Elixabet Sarasketa Zabala, **Project and Technology Transfer Manager,** MPC

Idoia Mugica Mendiola, **Outreach Manager,** MPC

Iker Landa Cunha, **Guest Student**

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

Laura Martín Montañez, **Outreach Internship,** MPC

María Formoso Ferreiro, **Administrative,** MPC

Marta López Pérez, **Administrative,** MPC

Txema Ramos Fernandez, **Administrative,** CSIC

Computing Services

Iñigo Aldazabal Mensa, **Computer Center Manager,** CSIC

Ioritz Paulis Garmendia, **IT Systems Technician,** MPC

Maintenance

Juan Manuel Burgos Jiménez, MPC

LABORATORY TECHNICIANS

Amaia Iturrospe Ibarra, CSIC

Luis Botana Salgueiros, CSIC

María Isabel Asenjo Sanz, MPC

María Lourdes Leza Fernández, UPV/EHU

Silvia Arrese-Igor Irigoyen, CSIC

Tamara Molina Rolo, MPC

Research Line:

Chemical Physics of Complex Materials

01 Gas/Solid Interfaces

Permanent Researchers

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

Post-doctoral Researchers

Alejandro Rivero Santamaria

Pre-doctoral Researchers

Alberto Rodríguez Fernández
Alfredo Serrano Jiménez
Auguste Tetenoire

Master Student

Maxime Infuso

Guest Researchers

Ivor Lončarić, Senior Scientist
Hua Guo, Senior Scientist
María Ángeles Hernández Vozmediano, Senior Scientist

02 Quantum Phenomena on Surfaces

Permanent Researcher

Nicolás Lorente Palacios, Scientific Researcher, CSIC

Ikerbasque Fellow

Deungjang Choi, MPC

Post-doctoral Researchers

Roberto Robles Rodríguez
Vladimir Zobac

Pre-doctoral Researchers

Cristina Mier González
José Reina Gálvez

Guest Researchers

Christoph Wolf, Post-doctoral Researcher
Fernando Delgado Acosta, Post-doctoral Researcher
Liliana Arrachea, Senior Scientist
María del Carmen Muñoz de Pablo, Senior Scientist
Paula Abufager, Senior Scientist
Young Rok Jang, Senior Scientist

03 Nanophysics Lab

Permanent Researchers

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

Post-doctoral Researchers

Andrew Weber
Djuro Bikaljevic
Ignacio Piquero Zulaica
Khadiza Ali
Laura Fernández Gómez-Recuero
Marco Gobbi
Maxim Ilin
Sara Barja Martínez

Pre-doctoral Researchers

Carmen González Orellana
Elia Turco
Fernando García Martínez
Marina Peña Díaz
Rodrigo Castrillo Bodero

Master Student

Afia Owusuah Akyaw

Undergraduate Students

Ane Telleria Lazcano
Borja Rodríguez Mateos
Irati Garmendia San Miguel

Guest Researchers

Javier García de Abajo, Senior Scientist
Naoya Sumi, Pre-doctoral Researcher
Tao Wang, Post-doctoral Researcher

04 Modelisation and Simulation

Permanent Researchers

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

Post-doctoral Researchers

Carlos García Fernández
Giuseppe Foti
Mikhail Otrokov
Pablo López Tarifa

Pre-doctoral Researchers

Emre Bölen
Carlos Corona García
Iker Gallardo Arrieta
Joseba Goikoetxea Perez
Masoud Mansouri
Moritz Müeller
Sophie Espert

Master Student

Sobodh Kumar

Guest Researchers

Aleksandra Viazovskaia, Pre-doctoral Researcher
Gustav Bihlmayer, Senior Scientist

05 Spectroscopy at Atomic Scale

Permanent Researcher

Lucia Vitali, Ikerbasque Professor, UPV/EHU

Post-doctoral Researchers

Anastasiia Riabishchenkova
Jie Hou

Pre-doctoral Researcher

Ana Barragán Durán

Undergraduate Student

Ninon Möhl

Research Line:

Electronic Properties at the Nanoscale

06 Electronic Excitations in Surfaces and Nanostructures

Permanent Researchers

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

Post-doctoral Researchers

Ilya Nechaev
Marta Pelc

Pre-doctoral Researchers

Jozef Janovec
Mikel Arruabarrena Larrarte
Raúl Guerrero Avilés

Guest Researcher

Magdalena Marganska, Post-doctoral Researcher

07 Quantum Theory of Materials

Permanent Researchers

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

Post-doctoral Researchers

Miguel Martínez Canales
Raffaello Bianco

Pre-doctoral Researchers

Antonella Meninno
Francesco Belli
Iñigo Robredo Magro
Martín Gutiérrez Amigo
Oscar Rodríguez Ballesteros
Pugeng Hou
Unai Aseguinolaza Aguirreche

Guest Researchers

Estelina da Silva, Post-doctoral Researcher
Jianqiang Zhou, Post-doctoral Researcher
José Flores Livas, Post-doctoral Researcher
Víctor García Suárez, Senior Scientist

08 Mesoscopic Physics

Permanent Researchers

Sebastián Bergeret Sbarbaro, Scientific Researcher, CSIC

Ikerbasque Associate

Vitaly Golovach, UPV/EHU

Post-doctoral Researchers

Claudio Guarcello
Stefan Ilic

Pre-doctoral Researchers

Alba Pascual Gil
Cristina Sanz Fernández
Julie Isabelle Baumard
Mikel Rouco Martin
Xian-Peng Zhang

Guest Researchers

Miguel Ángel Cazalilla Gutiérrez, Senior Scientist
Pauli Tapio Virtanen, Post-doctoral Researcher
Risto Ojajärvi, Pre-doctoral Researcher

09 Nano-Bio Spectroscopy

Permanent Researcher

Ángel Rubio Secades, University Professor, UPV/EHU

10 Souza Research Group

Permanent Researcher

Ivo Souza, Ikerbasque Professor, UPV/EHU

Post-doctoral Researcher

Julen Ibañez Azpiroz

Pre-doctoral Researcher

Miguel Ángel Jiménez Herrera

Guest Researchers

Cheol-Hwan Park, Senior Scientist
Stepan Tsirkin, Post-doctoral Researcher

11 Ceramic and Cement-Based Materials

Permanent Researcher

Jorge Sánchez Dolado, Tenured Scientist, CSIC

Post-doctoral Researcher

Guido Goracci

Guest Researchers

Albina Kostiuchenko, Pre-doctoral Researcher
Mohammadreza Izadifar, Pre-doctoral Researcher
Shizhe Zhang, Pre-doctoral Researcher
Valentina Musumeci, Pre-doctoral Researcher
Yun Chen, 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

Edurne Gorraitz Eusa
Luca Bergamini
Roberto Álvarez Boto
Tomas Neuman

Pre-doctoral Researchers

Alvaro Nodar Villa
Andrea Koneçna
Antton Babaze Aizpurua
Bruno Candelas Peñalba
Carlos Maciel Escudero

Guest Researchers

Annemarie Pucci, Senior Scientist
Garnett Bryant, Senior Scientist
Gilad Haran, Senior Scientist
Jack Peter Griffiths, Pre-doctoral Researcher
Juan Carlos Idrobo Tapia, Post-doctoral Researcher
Krzysztof Michal Czajkowsk, Pre-doctoral Researcher
Mario Zapata Herrera, Post-doctoral Researcher
Mikolaj Schmidt, Post-doctoral Researcher
Pedro Braña Coto, Post-doctoral Researcher
Tamás Földes, Post-doctoral Researcher
Yao Zhang, Post-doctoral Researcher

13 Nanomaterials and Spectroscopy

Permanent Researcher
Yuri Rakovich, Ikerbasque Professor, UPV/EHU

Post-doctoral Researcher
Thomas Hendel

Guest Researchers
Victor Krivenkov, Post-doctoral Researcher
Daria Diagileva, Master Student

14 Laser Physics and Photonic Materials

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

15 Quantum Nanophotonics Laboratory

Permanent Researcher
Gabriel Molina Terriza, Ikerbasque Professor, MPC

Post-doctoral Researcher
Juan José Miguel Varga

Pre-doctoral Researchers
Iker Gómez Viloria
Jon Lasa Alonso
Martin Molezuelas Ferreras

Master Students
Florian Lochon
Harriet Kumi

Guest Researchers
Iwo Bialynicki-Birula, Senior Scientist
Zofia Białynicka-Birula, Senior Scientist

Research Line:

Polymers and Soft Matter

16 Polymers and Soft Matter

Permanent Researchers
Angel Moreno Segurado, Tenured Scientist, CSIC
Ángel Alegría Loinaz, University Professor, UPV/EHU
Arantxa Arbe Méndez, Research Professor, CSIC
Daniele Cangialosi, Tenured Scientist, CSIC
Felix Fernández Alonso, Ikerbasque Professor, MPC
Fernando Álvarez González, Associate Professor, UPV/EHU
Gustavo 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

Ikerbasque Fellow
Jon Maiz Sancho
Paula Malo de Molina Hernández

Post-doctoral Researchers
Beatriz Robles Hernández
Daniel Enrique Martínez Tong
Daniel José Arismendi Arrieta
Luis Alejandro Miccio
María Ester Verde Sesto
Mohammad Ali Aboudzadeh Barihi
Xabier Gaetan Monnier

Pre-doctoral Researchers

Agustín Blazquez Martín
Amaia Matanza Corro
Ander Mendia Velasco
Javier Martínez Sabando
Jokin Pinacho Olaciregui
Jon Rubio Cervilla
Jordan Ochs
Jorge Humberto Melillo
Julen de la Cuesta Leone
Maiara Aime Iriarte Alonso
Mariarita Paciolla
Matteo Sanviti
Maud Formanek
Numera Shafqat
Thomas Louis Gambino

Undergraduate Students

Jon Ruiz Tarango
Iker Castrillo Maestro
Julen Olasagasti Imizcoz
Estibaliz Otegui Berrondo
Leire Orbegozo Pagobide

Guest Researchers

Carmen Mijangos Ugarte, Senior Scientist
Dieter Richter, Senior Scientist
Farihah Haque, Pre-doctoral Researcher
Helena Svajdlenkova, Post-doctoral Researcher
Jetro Epse Njukeng Nkengafac, Senior Scientist
José Luis Neira Faleiro, Senior Scientist
Jozef Bartos, Senior Scientist
Julian Oberdisse, Senior Scientist
Laura Álvarez Francés, Post-doctoral Researcher
Michelina Soccio, Post-doctoral Researcher
Rodney Dewayne Priestley, Senior Scientist
Timo Brändl, Post-doctoral Researcher

OTHER POSITIONS

Associate Professor

Isabel Tellería Echeverría, UPV/EHU

Scientific Researchers

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

Post-doctoral Researchers

Wen Wan, DIPC (Miguel Moreno Ugeda's group)
James Lawrence, DIPC (Dimas García de Oteyza's group)

Pre-doctoral Researchers

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

Undergraduate Student

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

EXTERNAL ADVISORY COMMITTEE

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
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.

Emeritus 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)* from 1989 to 2017; *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
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.

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.

RESEARCH LINES, GROUPS AND HIGHLIGHTS

RESEARCH LINE	GROUP	ACTIVITY
Chemical Physics of Complex Materials	01 Gas/Solid Interfaces	Theoretical
	02 Quantum Phenomena on Surfaces	Experimental and 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 Quantum Theory of Materials	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.

In 2019, Ikerbasque professor Félix Fernández Alonso joined the Polymers and Soft Matter research line at CFM to reinforce the use of neutron techniques in the characterization of materials.

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 (01), the "Quantum Phenomena on Surfaces" group (02), and the "Modelisation and Simulation" group (04). 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" (03) and the "Spectroscopy at Atomic Scale" (05) groups.

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

01 Gas/Solid Interfaces

Group Leader: Ricardo Díez Muiño, Scientific Researcher, CSIC

The "Gas/Solid Interfaces" group is focused on understanding the elementary reactive processes that may happen whenever atoms or small molecules interact with surfaces at the atomic scale. When a molecule approaches the surface, intramolecular chemical bonds can break down and new ones be formed with the surface. Reliable simulations of these complex phenomena are performed by combining first-principles electronic structure calculations, which describe the details of the interaction between the gas species and the surface, with high-dimensional classical equations of motion of the nuclei. Particular attention is paid in developing theoretical models to treat the non-adiabatic processes and the energy dissipation channels that come into play, because they can drastically change the output of the dynamics. More recent lines of research also include development of theoretical methods to describe photo-induced adsorbate dynamics and reactions, as well as machine learning methods specific for the gas/solid interface dynamics.

02 Quantum Phenomena on Surfaces

Group Leader: Nicolás Lorente Palacios, Scientific Researcher, CSIC

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 solid surfaces, ranging from semiconductors and metals to superconductors. 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. Dr. Deung-Jang Choi leads the experimental work and Dr. Nicolas Lorente leads the theoretical work.

03 Nanophysics Lab

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

The NanoPhysics Lab (NPL) group studies structural, electronic, magnetic and chemical properties of in-situ and ex-situ grown nanostructures, in the context of experimental surface science. NPL aims at exploring relevant but yet-widely-unknown phenomena taking place at the surface of solid materials, such as the atomic-level control of on-surface chemical reactions and catalysis, the bottom-up fabrication of 1D or 2D functional materials, and also the growth of novel layered materials with potential application in state-of-the-art technology devices. It is also worth to mention the exploration of such surface properties and phenomena using curved crystals of varied nature as substrates, defining a radically new experimental approach that is becoming the hallmark of the group. The NPL holds some of the most modern and complete set of surface-sensitive techniques and instrumentation, combined in a variety of multi-technique ultra-high-vacuum setups, and distributed in five different laboratory rooms.

04 Modelisation and Simulation

Group Leader: Daniel Sánchez Portal, Research Professor, CSIC

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 (STM) images and tunneling spectroscopies. The group has also been devoted to the study of the 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.

05 Spectroscopy at Atomic Scale

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

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 focuses 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, (iii) the investigation of new strategies leading to the formation of covalently bonded conjugated structures with functional groups, and (iv) two dimensional properties emerging in layered materials.

The experimental research activity is based on a low temperature scanning probes microscope, which is used to correlate structure, electronic and vibrational properties of nanostructures and interfaces at the atomic scale. The growth of the interfaces as well as their characterization take place in ultra-high vacuum and at temperatures down to 1K, a challenging situation from the methodological point of view.

HIGHLIGHT

Strong synergy between hot-electrons and phonons rules the photo-induced desorption of CO from Pd (111)

Alducin M, Camillone III N, Hong SY, and Juaristi JI.

Physical Review Letters 123, 246802 (2019)

Ultrafast laser pulses in the ultraviolet, visible, and near-infrared are extremely efficient in promoting a variety of surface adsorbate dynamical processes, including diffusion, desorption, and reactions. Irradiation of a metal surface with large laser fluences (~1mJ/cm^2) generates a transient nonequilibrium distribution of hot electrons, which rapidly thermalize into a Fermi-Dirac distribution with an electron temperature of several thousand Kelvin that largely exceeds the lattice temperature. Subsequently, the photon-excited electronic system can transfer energy directly to the adsorbate, but also indirectly via the vibrationally excited surface lattice that results from electron-phonon coupling.

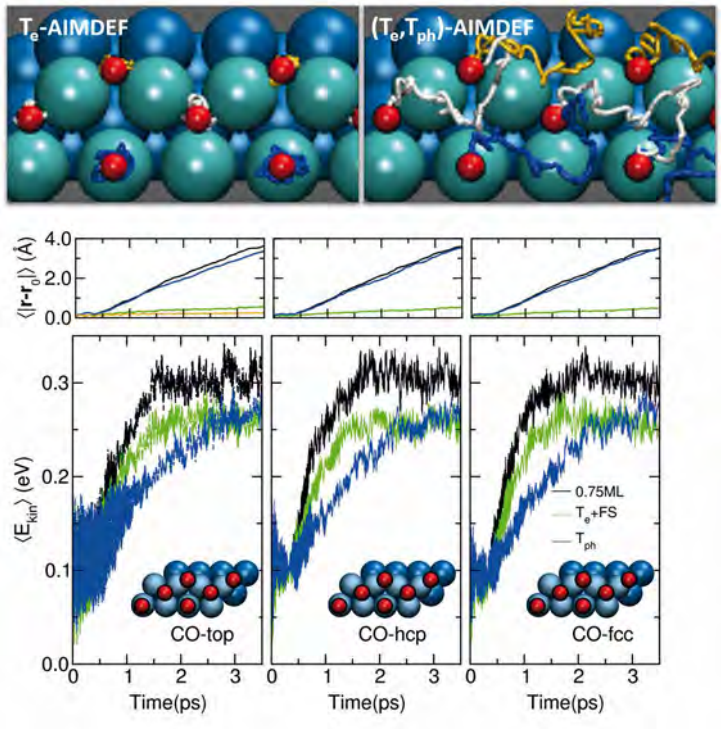
Two-pulse correlation (TPC) experiments are usually employed to establish the timescale of the adsorbate-substrate energy transfer and, accordingly, determine whether the adsorbate reaction is electron or phonon mediated. Most systems investigated so far are characterized by time responses of a few picoseconds or less that are ascribed to a dominant electron-assisted process [5–9]. Only the desorption of CO from Ru (0001), with a TPC time response of ~20 ps, is considered to be phonon dominated. Thus, it is fair to conclude that the role of the electron-excited phonons has generally been overlooked; due in part to the lack of a theoretical model advanced enough to incorporate all the ingredients in this complex scenario.

In this letter, the authors propose a novel ab initio classical dynamics scheme that incorporates effects due to the photon-excited electronic and phononic systems, as well as out-of-phase coadsorbate dynamics. Using this complete dynamics, it is now possible to demonstrate that both electrons and phonons are critical to understanding the ultrafast desorption dynamics of CO from Pd (111).

By performing different types of simulations in which electrons and phonons are alternatively switched on and off, the authors are able to disentangle the contribution of the heated electronic and phononic systems in the desorption dynamics. Specifically, hot electrons efficiently couple energy into CO translational degrees of freedom while hot phonons reduce the CO-Pd bond strength by destabilizing the adsorbed CO from its equilibrium positions. The latter can be inferred by comparing the time evolution of the CO displacements obtained when the excited phonons are or not included

in the simulations (middle panels in the figure). As a result, the hot electrons are more efficient in desorbing the phonon-induced unstable CO molecules. The CO trajectories sketched in the top panels when only hot electrons (left panel, T_e-AIMDEF) and both electrons and phonons (right panel, (T_e,T_{ph})-AIMDEF) contribute are good examples of how the excited phonons affect the CO dynamics at 0.75 ML.

Altogether, this theoretical study provides a renewed perspective on the importance of phonons in promoting the electron-mediated femtochemistry of adsorbates at metals.



Top: *Examples of typical CO trajectories in T_e-AIMDEF (left) and (T_e, T_{ph})-AIMDEF (right) simulations for 0.75 ML-CO/Pd(111).* Bottom: *Site-resolved mean kinetic energy of the nondesorbing CO against time for 0.75ML coverage: top CO (left panel), hcp CO (middle panel), and fcc CO (right panel). Results obtained from (T_e, T_{ph})-AIMDEF (black), Te-AIMDEF (green), and T_{ph}-AIMD (blue).* Middle: *Mean distance of the nondesorbing-CO geometrical center with respect to its initial position. Color criteria and ordering of panels as in bottom figures.*

HIGHLIGHT

Atomic-scale spin sensing with a single molecule at the apex of a scanning tunneling microscope

Verlhac B, Bachellier N, Garnier L, Ormaza M, Abufager P, Robles R, Bocquet ML, Ternes M, Lorente N and Limot L

Science 366, 623-627 (2019)

An international team led by Laurent Limot (Strasbourg), Markus Ternes (Jülich) and Nicolás Lorente, researcher at CFM and the Donostia International Physics Center (DIPC) has shown that minute magnetic fields can be detected using a magnetic molecule that is scanned along a surface. The scanning is made displacing the molecule on a metallic tip such that the displacements are sub-atomic and an electronic current is passed between the tip and the studied substrate. The small displacements are key to obtaining very high resolution but the new aspect of the work is to use a magnetic excitation of the molecule when electrons flow through it. The magnetic excitation can easily be perturb by the substrate yielding precious information on its magnetic structure.

The authors of the recent publication in Science specially crafted the tip apex to bring a novel function to the sharp tip: They made it sensitive to magnetic moments by placing a quantum molecular magnet containing a single Nickel atom. The molecule is shown in the figure in the configuration gleaned from geometrical studies mainly using calculations. The ground state of the molecule corresponds to a molecular magnetic moment parallel to the substrate surface. The molecule has a low-energy excitation of roughly 4 meV that corresponds to directing the magnetic moment perpendicular to the surface. The spin of this molecule is S=1 and is preserved in the depicted configuration. The excitation is easily performed by the flowing electrons in the figure's set up because each electron efficiently undergoes a spin flip while exciting the molecular spin, to preserve the system's total spin. The excitation opens a new conduction channel leading to a jump in the differential conductance of the molecular junction that is revealed in the measurements. This jump takes place at the bias matching the excitation energy. When the molecule is close to a magnetic object, the excitation energy changes due to the new magnetic excitations. As a consequence, the magnetic properties of the surface can be studied with sub-atomic resolution.

There are two important aspects of this work. First, the use of a molecule as active sensor makes it very reproducible and easy to implement in instruments used by other groups working in the field worldwide. Second, the detection scheme relies only on easily observable properties in the sensor tip and "dark" magnetic moments, which are usually difficult to measure, become accessible. In summary, with this work scientists have expanded their nanoscale toolbox with a new tool sensitive to the magnetic properties, which will be important for future applications ranging from nanoscale memory-devices to novel materials or applications in the field of quantum simulation and computing.

> A molecule at the tip of the tunneling microscope is the key to achieving unprecedented accuracy of magnetic detection on an atomic scale.

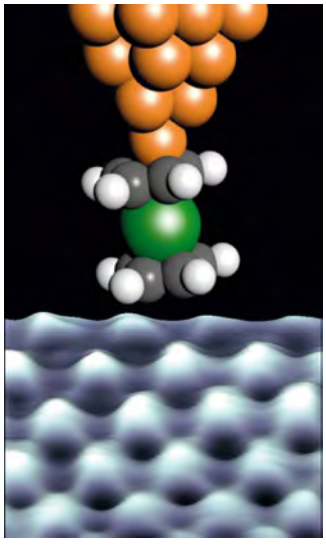


Figure: *Atomic scheme of a nickelocene molecule (atoms gray for carbon, white for hydrogen and green for nickel) attached to a single-atom terminated scanning tunneling microscope tip (orange atoms for copper). The lower part of the figure shows the differential conductance at the molecular tip scans the surface. The conductance shows atomic resolution of the different magnetic atoms (cobalt in the present case) showing that this technique can be used to learn about the spatial distribution of atomic magnetic moments.*

HIGHLIGHT 1

Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides

Barja S, Refaely-Abramson S, Schuler B, Qiu DY, Pulkin A, Wickenburg S, Ryu H, Ugeda MM, Kastl C, Chen C, Hwang C, Schwartzberg A, Aloni S, Mo SK, Ogletree DF, Crommie MF, Yazyev OV, Louie SG, Neaton JB, and Weber-Bargioni A

Nature Communications 10, 3382 (2019)

Atomically thin, two dimensional (2D) semiconductors known as transition metal dichalcogenides (TMDs) are not perfect, but their imperfections can actually be a good thing. Crystal defects are known to modify semiconductor functionality and are expected to have particularly strong impact on the properties of 2D materials, where screening is reduced compared to bulk systems. In particular, 2D-TMDs can feature a variety of different defect geometries and related electronic states. Understanding how defects are structured at the atomic scale, how they are created, and how they interact with electrons are the first steps to designing new advanced materials. However, the experimental identification of individual defects and the direct correlation of these measurements to their electronic structure is far from simple.

In the world of materials science, many researchers assumed that the most abundant defects in TMDs were the result of missing atoms or "vacancies" of sulfur in tungsten disulfide (WS_2), or selenium vacancies in molybdenum diselenide ($MoSe_2$). These missing S or Se atoms are predicted by theory to locally alter the electronic structure of the semiconductor by introducing deep in-gap states (IGS). Consequently, important features in the experimental transport characteristic, optical response and catalytic activity of 2D-TMDs have typically been attributed to chalcogen vacancies, based on indirect support from images acquired by transmission electron microscopy (TEM) and scanning tunneling microscopy (STM). Still, there are a variety of technical challenges that limit the direct correlation of the former atomic scale studies on TMD materials with their macroscopic response, leading to a non-consistent interpretation of the defect type across the current literature.

But as reported in Nature Communications, the defects previously observed with other methods are actually created by oxygen atoms replacing sulfur or selenium atoms, instead of pristine chalcogen vacancies. Oxygen, like sulfur and selenium, is part of the oxygen or "chalcogen" family of elements. Moreover, since chalcogens share similar properties, there is not much change in electronic states of the semiconductor with such replacement: oxygen substituted in the chalcogen sublattice does not form deep in-gap states.

Key to this finding was the use of a non-contact atomic force microscope (nc-AFM), with a single carbon monoxide (CO) molecule acting as an ultrasharp "tip" or probe, combined with a scanning tunneling microscope (STM). When used with AFM, the CO-tip images the surface atoms at a very high resolution inaccessible with conventional techniques, which helps to identify the defect's atomic site. Direct correlation to the defect's unique electronic fingerprint was achieved by parallel scanning tunneling microscopy and spectroscopy measurements on the very same defect. These experimental efforts, together with parallel state-of-the-art first-principles ground- and excited-state calculations using density functional theory (DFT) and many-body perturbation theory within the GW approach, respectively, had enabled an unprecedented interrogation of the system.

Direct correlation between the atomic and electronic structures of individual defects in 2D-TMDs is required to achieve a fundamental understanding of the effect of defects on the electronic structure of the material. This work directly relates atomic and electronic structure through combined nc-AFM and STS measurements of individual point defects in monolayer $MoSe_2$ grown by molecular beam epitaxy and in monolayer WS_2 grown by chemical vapor deposition. Although nc-AFM and STM images of chalcogen defects appear to be consistent with vacancies, a comparison with DFT and GW calculations establishes these defects as substitutional oxygen at chalcogen sites, consistent with the lack of IGS in the band structure. Therefore, the comprehensive joint experimental and theoretical study reveals substitutional oxygen as a prolific point defect in 2D-TMDs and provides critical insight for future defect engineering in these systems.

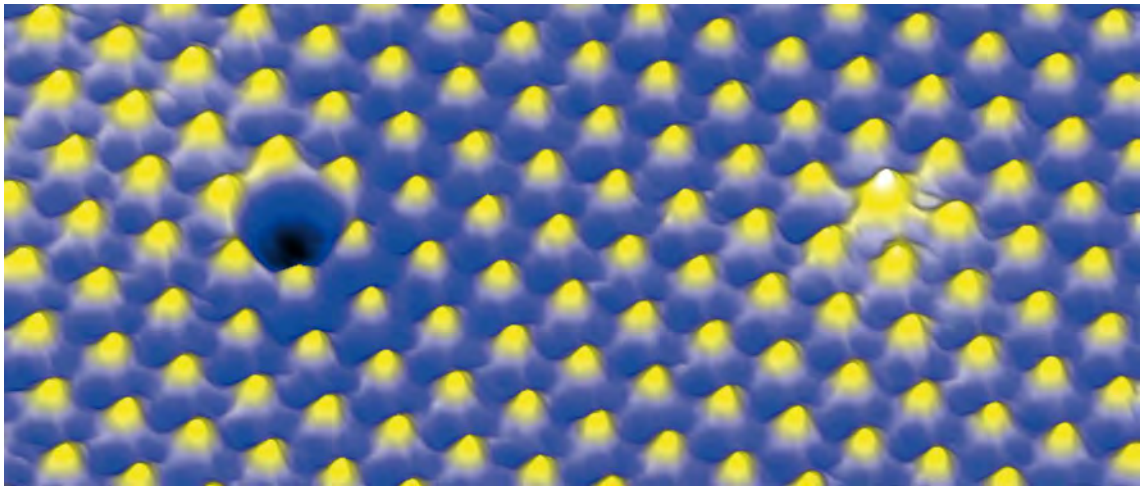


Figure: *Atomic force microscopy image (temperature 4K) of two oxygen atoms replacing selenium atoms in molybdenum disulfide. The oxygen in the left defect replaces a selenium atom in the upper selenium layer, facing the "tip", and appears as a depression in the lattice. The oxygen in the right defect replaces a selenium atom in the bottom selenium layer, opposite the "tip", and slightly pushes the selenium atom upward relative to the pristine lattice.*

HIGHLIGHT 2

Near-infrared plasmons with atomically thin crystalline silver films

Abd El-Fattah ZM, Mkhitaryan V, Brede J, Fernández L, Li C, Guo Q, Ghosh A, Rodríguez Echarri A, Naveh D, Xia NF, Ortega JE, and García de Abajo.

ACS Nano 13, 7771 (2019)

An international team of researchers demonstrates the existence of narrow plasmons in the near-infrared regime by using atomically-thin silver films of crystalline quality.

Even though we might not be aware of it, plasmons in noble metals, such as silver and gold, have been used to color glass since ancient times. In recent years, ***plasmonics*** has made its way through to become a key component in the field of optical devices essential in the miniaturization of optoelectronic devices to the nanoscale.

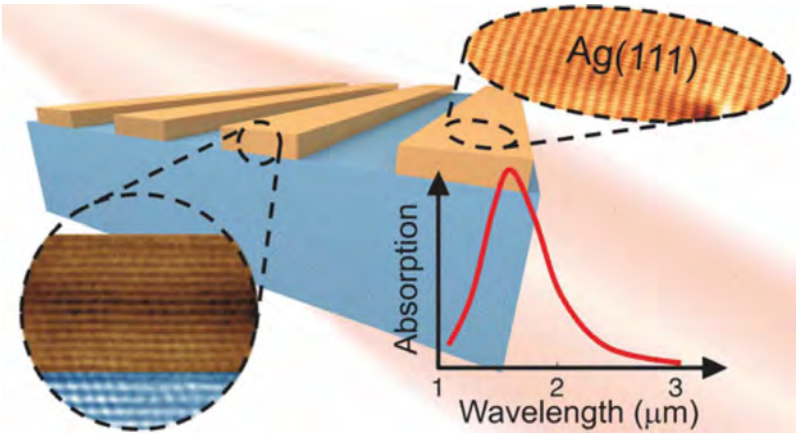


Figure: *Schematic description of the Ag nanostripe array. Transmission Electron Microscopy (left) and Scanning Tunnelling Microscopy (top) provide direct proof of the atomic perfection across the interface and at the very surface, respectively. Such atomic sharpness provides a powerful way of tuning plasmon excitations in the near-infrarred region of the spectrum.*

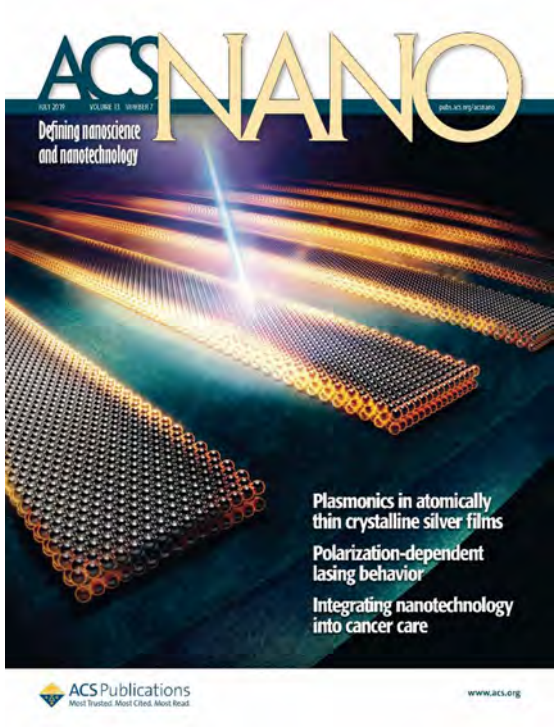
It is known that plasmonic interactions between electrons and photons change significantly in materials when one or more of the dimensions of the metallic object are reduced down to the nanometer scale. The advent of graphene and other two-dimensional crystals has helped display appealing properties of plasmons such as a large electrical tunability. However, the plasmons generated in these materials are too broad or exist at too low frequencies, in a range that is well below the expected near-infrared regime needed for most optical devices.

In this study, published in ACS Nano and selected to appear as the cover image of the July journal issue, researchers from ICFO, together with Jens Brede, Laura Fernández and Enrique Ortega from CFM and DIPC, and other collaborators from Yale University and Bar Ilan University, report on the fabrication and the excellent plasmonic and electronic properties of wafer scale atomically thin crystalline silver films composed of only a few atomic layers.

Through a two-step process of fabrication and under ultrahigh-vacuum conditions, the team of researchers was able to grow high-quality flat silver Ag (111) films on silicon Si (111) wafers, with a thickness as small as ~1.5nm (equivalent to seven atomic monolayers). The film quality was high enough to resolve quantum electronic states through angle-resolved photoemission. To excite and probe plasmons in these films, they first carved nanoribbon arrays, and then shinned near-infrared light. Narrow plasmons with high quality factor (~4) were observed as spectral features in the reflected and transmitted light.

The results of this study prove that atom-thin crystalline silver films are capable of supporting high-quality narrow plasmons in the near infrared, below ~2 micron wavelength. In addition, this study has proven that such material could be the perfect alternative to highly-doped graphene, which, despite its amazing properties, has only reached the mid-infrared (wavelengths above ~5 microns), far from the technologically attractive near-infrared region.

The observation of these spectrally sharp and strongly confined plasmons in atomically thin silver holds great potential for electro-optical modulation and optical sensing applications.



Cover of ACS Nano

HIGHLIGHT 1

Antiferromagnetic topological insulator $MnBi_2Te_4$

Otrokov MM, Klimovskikh II, Bentmann H, Estyunin D, Zeugner A, Aliev ZS, Gass S, Wolter AUB, Koroleva AV, Shikin AM, Blanco-Rey M, Hoffmann M, Rusinov IP, Vyazovskaya AY, Eremeev SV, Koroteev YM, Kuznetsov VM, Freyse F, Sanchez-Barriga J, Amiraslanov IR, Babanly MB, Mamedov NT, Abdullayev NA, Zverev VN, Alfonsov A, Kataev V, Buchner B, Schwier EF, Kumar S, Kimura A, Petaccia L, Di Santo G, Vidal RC, Schatz S, Kissner K, Unzelmann M, Min CH, Moser S, Peixoto TRF, Reinert F, Ernst A, Echenique PM, Isaeva A, and Chulkov EV.

Nature 576, 416 (2019) [1]

Otrokov MM, Rusinov IP, Blanco-Rey M, Hoffmann M, Vyazovskaya AY, Eremeev SV, Ernst A, Echenique PM, Arnau A, and Chulkov EV.

Physical Review Letters 122, 107202 (2019) [2]

Ever since the discovery of topologically-nontrivial materials, a magnetically ordered phase in an insulating compound had never been observed to coexist with such a type of electronic order as a topological insulator state. In these recent studies, the authors report on this kind of electronic behavior in the $MnBi_2Te_4$ compound, which turns out to be an intrinsic antiferromagnetic topological insulator.

Magnetic topological insulators are narrow-gap semiconductor materials that combine non-trivial band topology and magnetic order. Unlike their nonmagnetic counterparts, magnetic topological insulators may have some of the surfaces gapped due to breaking of the time-reversal symmetry, which enables a number of exotic phenomena with potential applications in spintronics. So far, magnetic topological insulators have only been created by means of doping nonmagnetic topological insulators with 3*d* transition metal elements. However, such an approach leads to strongly inhomogeneous magnetic and electronic properties of these materials, restricting the observation of important effects to very low temperatures. Finding an intrinsic magnetic

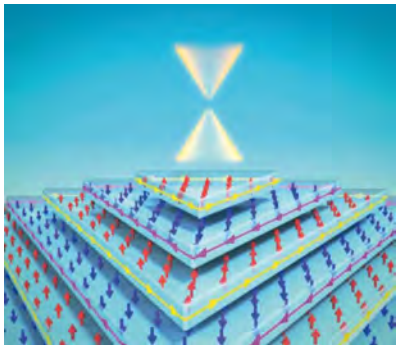


Figure: *Artistic representation of the stepped surface of $MnBi_2Te_4$ with the characteristic electronic feature of a magnetic topological insulator (the so-called Dirac Cone) shown above. The red and blue arrows refer to the local magnetic moments of the Mn atoms, which show alternate directions from one terrace to the next, i.e., antiferromagnetic order. The yellow and pink lines, as well as their respective arrows show the directions of propagation of the electric currents at the edges, which are opposite between neighboring edges (this is known as half-integer quantum Hall effect).*

> The antiferromagnetic topological insulator $MnBi_2Te_4$ is a unique platform allowing the realization of at least four different quantum Hall effects, some of which have already been observed very recently.

topological insulator, i.e. a stoichiometric well-ordered magnetic compound, could be an ideal solution to these problems, but no such material has been observed to date. In a recent work by the group[1], using density-functional theory, the authors predict and further confirm by means of structural, transport, magnetic, angle- and spin-resolved photoemission spectroscopy measurements the realization of the antiferromagnetic topological insulator phase, which is hosted by the van der Waals layered compound $MnBi_2Te_4$. An interlayer antiferromagnetic ordering makes $MnBi_2Te_4$ invariant with respect to the combination of the time-reversal (Θ) and primitive-lattice translation ($T_{1/2}$) symmetries, $S = \Theta T_{1/2}$, giving rise to the Z_2 topological classification of antiferromagnetic insulators. They find $Z_2 = 1$ for $MnBi_2Te_4$, which confirms its topologically nontrivial nature. The S-breaking (0001) surface of $MnBi_2Te_4$ exhibits a giant band gap in the topological surface state, as evidenced by ***ab initio*** calculations and photoemission measurements. These results culminate almost a decade-long search of an antiferromagnetic topological insulator, the possible existence of which having been predicted in 2010. In a broader sense, $MnBi_2Te_4$ is the first intrinsic magnetic topological insulator realized experimentally.

In the two-dimensional limit, $MnBi_2Te_4$ is predicted [2] to show a unique set of thickness-dependent magnetic and topological transitions, which drive it through ferromagnetic and (un)compensated antiferromagnetic phases, as well as quantum anomalous Hall state and its zero plateau. Thus, $MnBi_2Te_4$ is the first stoichiometric material predicted to realize the zero-plateau quantum anomalous Hall state intrinsically. This state was earlier predicted to host the axion insulator phase.

The discovery of the first antiferromagnetic topological insulator opens a new field of magnetic topological insulators that focuses on intrinsically magnetic stoichiometric compounds. As an outcome of this, a number of fundamental phenomena are expected to be eventually observed, such as quantized magnetoelectric coupling and axion electrodynamics. Other exotic phenomena could become accessible at temperatures significantly higher than those achieved to date, like the quantum anomalous Hall effect and chiral Majorana fermions.

> The quantum effects featured by $MnBi_2Te_4$ are potentially useful for the development of a new generation magneto-electronic devices.

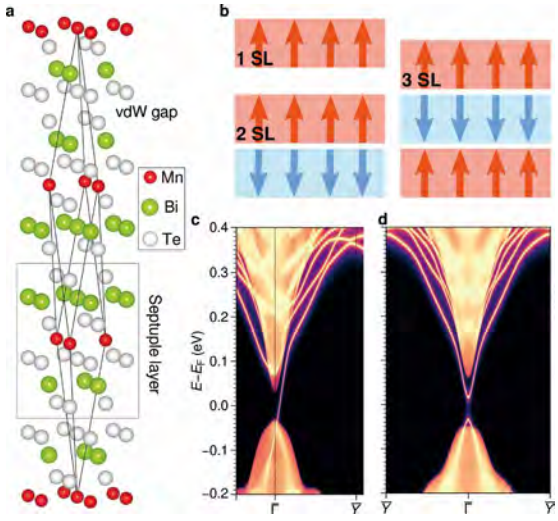


Figure: *(a) Atomic structure of $MnBi_2Te_4$ with red, green, and white balls showing Mn, Bi, and Te atoms, respectively. (b) 1-, 2-, and 3-septuple-layer(SL)-thick $MnBi_2Te_4$ films, showing a ferromagnetic, compensated antiferromagnetic, and uncompensated antiferromagnetic orders, respectively. (c,d) Edge electronic band structures of the MnBi2Te4 2-SL-thick film calculated for the ferromagnetic (c) and compensated antiferromagnetic (d) states. The presence of the edge mode in the fundamental band gap of the film (c) indicates the QAH phase, while the gapped edge spectrum (d) is a proof of the zero plateau QAH state.*

HIGHLIGHT 2

Electronic transport in planar atomic-scale structures measured by two-probe scanning tunneling spectroscopy

Kolmer M, Brandimarte P, Lis J, Zuzak R, Godlewski S, Kawai H, Garcia-Lekue A, Lorente N, Frederiksen T, Joachim C, Sanchez- Portal D, and Szymonski M.

Nature Communications 10, 1573 (2019)

Miniaturization of electronic circuits into the single-atom level requires novel approaches to characterize transport properties. Since its invention by Binnig et al. in 1982, the scanning tunneling microscope (STM) is regarded as the method of choice for real-space imaging of the electronic structure of conducting surfaces with picometer resolution. Single-probe STM is also a spectroscopic tool, able to locally probe electronic surface states as a function of the bias voltage in the scanning tunneling spectroscopy (STS) mode. Furthermore, the precision reached in approaching the STM tip apex toward the surface permits for a controlled electronic contact with a single surface atom or molecule.

However, direct determination of the electronic transport properties of a planar atomic-scale wire or circuit lies beyond the single-probe approach. Such characterization requires fabricating metal contacts with high precision, which is usually a challenge. An attractive alternative is the use of multi-probe STM. This method offers high control on the position and geometry of the contacts between the probes and the nanoscale system. But the downscaling of multi- probe instruments toward the atomic level, ***i.e.,*** where all STM tip apex positions are controlled at the atomic scale, meets many technical obstacles. Although two-probe STM (2P-STM) experiments have been proposed already in the nineties, practical implementations of those propositions were not feasible. The main obstacle was the insufficient stability that caused a lack of both atomic precision in relative probe-to-probe positioning and picometer precision in probe-to-sample contact determination. In fact, only recently 2P-STM experiments have reached the required atomic precision in contacting structures on a surface, however no experimental protocols for extracting transport properties of atomic structures from such experiments had been reported.

An international team of researchers, including members from CFM and DIPC, used for the first time a 2P-STM/STS with probes operating in tunneling conditions over the same atomic- scale system to extract detailed information of in-plane electronic transport.

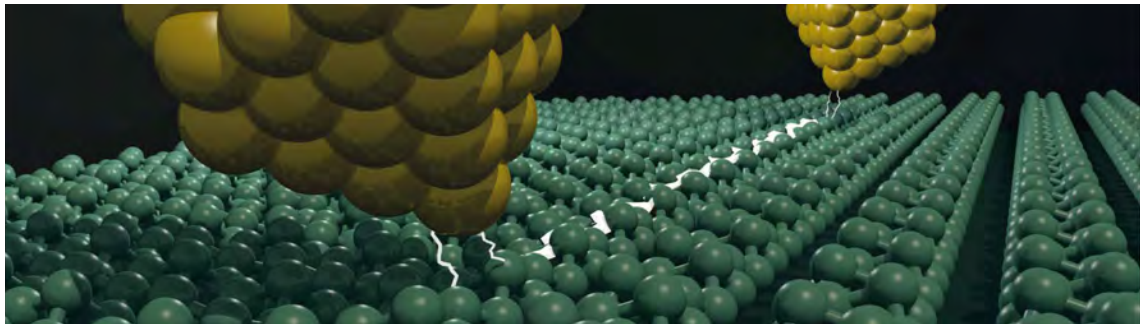


Figure 1: *Artistic view of the 2P-STM operating on Ge(001)-c(4x2). White lines represent electrons transmitted from one tip to the other through the quasi-one-dimensional surface states.*

They introduced a new method for the determination of the transconductance and demonstrate how it captures energy-resolved information about electronic transport through the unoccupied states from the anisotropic germanium (001) surface. Combining the new experimental protocol with state-of- the-art first-principles calculations they showed that 2P-STS brings information about coherent hot electrons transport in quasi-one-dimensional surface states of germanium (001).

The Ge(001) surface consists of buckled Ge dimers forming well-separated parallel rows. The existence of surface dangling bonds introduces additional unoccupied states within the band-gap of the bulk Ge electronic structure. Importantly, weak interactions between adjacent rows result in strong anisotropy of this band structure. Consequently, the reconstructed dimer rows on the bare Ge(001) surface form a series of parallel quasi-1D wires.

In the experiment, electrons injected from one STM tip are collected at a different location at a nanometric distance (down to 30 nm). This was theoretically modeled by a system composed of a twelve-layer Ge(001)-c(4×2) slab contacted by Au tips (Fig. 1). On this self-consistent 4-terminal treatment, two Ge electrodes were connected at each slab termination and other two at the Au model tips. A remarkable agreement was found between the calculated transmis- sion function and the experimental transconductance spectra. The sequential opening of two transport channels within the quasi-one-dimensional Ge dimer rows in the surface gives rise to two distinct resonances in the transconductance spectroscopic signal. These breakthrough simulations also elucidated the transport directionality of the injected hot electrons, revealing a transition from 2D to quasi-1D coherent transport regime.

This work demonstrates that complex experiment setups combined with advanced calcu- lations can provide new insights into transport properties at the nanoscale. The presented techniques are promising and applicable to characterize the quantum transport in 2D materials in general (graphene and beyond). In contrast to standard metal contacts, ***e.g.,*** fabricated by lithographic techniques, the use of 2P-STM enables a precise adjustment of individual atomic contacts and their resistances, allowing to access the system's intrinsic transport properties, disentangling them from those of the contacts and leads.

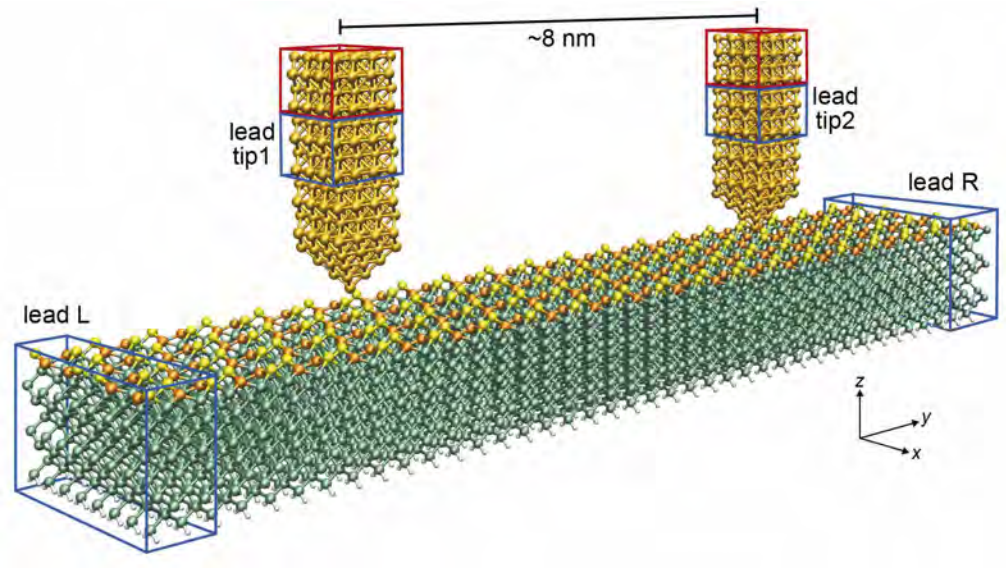


Figure 2: *First-principles transport simulations for the two-probe experiments, represented by a four-terminal setup. The electrode regions are highlighted by blue boxes, two of them located at each Ge(001)-c(4×2) slab terminations and the other two at each Au model tip.*

HIGHLIGHT

Can Atomic Buckling Control a Chemical Reaction? The Case of Dehydrogenation of Phthalocyanine Molecules on $GdAu_2$/Au (111)

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

Journal of Physical Chemistry C 123, 6496 (2019)

The efficiency of chemical reactions on surfaces is traditionally related to the atomic structure and catalytic activity of the substrate. Periodic out-of-plane lattice distortions of supported two-dimensional layers is an alternative strategy to promote reactions, strategy that has been scarcely investigated, so far. Here, the authors show that the variable buckling geometry of a $GdAu_2$ Moiré overlayer supported on the Au (111) surface exposes specific single-atom sites that trigger the selective dehydrogenation process of phthalocyanine (H2-PC) molecules. However, a reaction limit to about 1/3 of the monolayer is observed. This self-limited reaction can be explained considering the lattice mismatch between the substrate and the alloy layer, which leads to the previously reported outward displacement of distinct Gd sites.

The detailed knowledge of the surface atomic structures able to promote chemical reactivity is of paramount importance for solid-state nanochemistry. In this work, Vitali et al show that the loss of surface planarity observed in two-dimensional (2D) systems increases significantly the adsorption selectivity and additionally controls the surface chemistry. Specifically, the authors have characterized the reactivity of H_2-phthalocyanine (H2-PC) molecules adsorbed on periodic structures characterized by atomic-buckling. The periodic displacement of single atoms orthogonally to the surface plane shown by the $GdAu_2$/Au (111) surface develops spontaneously due to the not commensurable periodicity of the two interfaced structures. Thus, this system is characterized by variable lattice deformations, which reflect the local atomic interaction with the underlying surface. Specific single-atom sites are exposed, allowing them to explore the relationship between the dehydrogenation reaction of the H2-PC molecules and the atomistic structure of the supporting layer. We have demonstrated that this atomic displacement of the Gd atoms in the $GdAu_2$/Au (111) system naturally promotes site selectivity and specificity of the chemical reactions. The energetics of a dehydrogenation reaction of the H2-PC molecules is indeed related to the degree of atomic buckling.

By means of scanning tunneling microscopy, X-ray photoemission spectroscopy (XPS), and density functional theory (DFT) calculations, this work gives evidence that

the vertical displacement of the Gd atoms is responsible for the dehydrogenation of the macrocycle of only site-selected H2-PC molecules. Thus, at most, one-third of the monolayer (ML) of adsorbed molecules, corresponding to H2-PC molecules occupying well-defined positions of the Moiré superlattice, undergoes a dehydrogenation reaction. The H2-PC dehydrogenation strengthens the Gd–N interaction inducing structural relaxation effects in the alloy geometry. The deformation of this atomistic order may have possible consequences for the stability of the reported in-plane ferromagnetic character of the alloy layer. The present work provides valuable perspective in the selective activation of chemical reactions on surfaces. As atomistic buckling has been commonly reported on several two-dimensional systems, observed as Moiré patterns, the authors believe that these findings might apply generally.

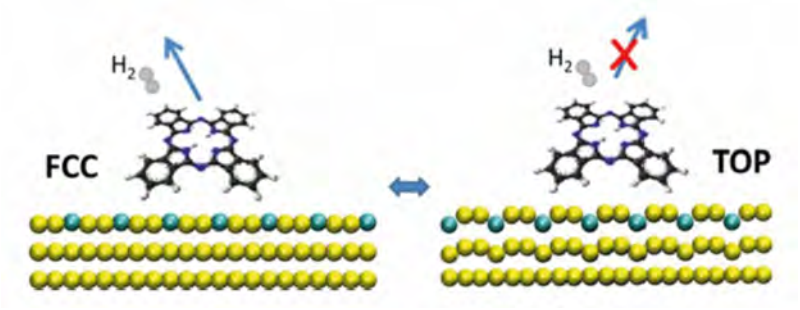


Figure: *Sketch of the dehydrogenation reaction of the H2-PC macrocycle according to specific corrugation of the $GdAu_2$/Au (111) system. Only when the Gd atoms buckle towards the vacuum region can promote the bonding to the nitrogen atoms of the H2-PC molecule, triggering their dehydrogenation.*

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. 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:

06 Electronic Excitations in Surfaces and Nanostructures

Group Leader: Andrés Ayuela Fernández, Scientific Researcher, CSIC

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

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.

07 Quantum Theory of Materials

Group Leader: Ion Errea Lope, Assistant Professor, UPV/EHU

The activity of the "Quantum Theory of Materials" group focuses on the first-principles calculation of materials properties and the development of new ab initio techniques. The group develops new theoretical methods to overcome the problems associated to standard theoretical approaches, specially, to describe with improved accuracy the quantum description of the electron-phonon and phonon-phonon interactions. These new techniques are applied to understand the electronic and vibrational properties of complex materials as well as to predict new compounds with interesting properties fully ab initio.

In the last years the team has concentrated its efforts to study (i) high-temperature superconducting hydrogen-based compounds at high pressure, as well as hydrogen itself; (ii) thermoelectric and charge-density wave materials both in the bulk and the monolayer, aiming at characterizing their phase diagram and their transport properties; (iii) collective electronic excitations in metals; and, finally, (iv) optical lattices.

In 2019, Ion Errea, a researcher from the University of the Basque Country (UPV/EHU) became the new leader of the group at CFM, taking care of the duties finely assumed by Aitor Bergara in Leioa over the last years.

08 Mesoscopic Physics

Group Leader: Sebastián Bergeret Sbarbaro, Scientific Researcher, CSIC

The activity of the "Mesoscopic Physics" group is devoted to the theoretical study of the quantum transport properties of nanostructures and mesoscopic systems. The research covers a wide variety of materials and structures including metals, ferromagnets, semiconductors, superconductors, low dimensional systems and topological matter. In addition to the purely theoretical activity, the group has a large network of experimental collaborators. In the past years special emphasis is placed on following research objectives: (i) to develop theoretical tools for studying spin-dependent transport in hybrid systems with different material combinations, (ii) to study the electronic heat transport at the nanoscale, (iii) to explore the possibility of using superconducting materials for bolometry, (iv) to design building blocks with new functionalities for quantum circuits and nanodevices.

09 Nano-Bio Spectroscopy

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

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, and (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).

10

Souza Research Group

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

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.

11

Ceramic and Cement-Based Materials

Group Leader: Jorge Sánchez Dolado, Tenured Scientist, CSIC

The group researches a variety of properties of cement-based and ceramic materials experimentally and theoretically. 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 CO2 fingerprint. The initial objectives of the group are: (i) the use of atomistic and colloidal simulations to study the structure and properties of cement-based materials, (ii) the implementation of new hydrothermal and supercritical fluids (SCF) technologies for the ultra-fast synthesis of ceramic nanoparticles, (iii) the development of new sintering methodologies through the use of autoclaves or microwaves that allow notable energy savings and a drastic reduction of CO2 emissions, and (iv) the development of energy storage solutions based on cement-based materials, including both chemical storage (batteries) and thermal storage systems (TES) applications.

HIGHLIGHT

Self-assembled triangular graphene nanostructures

Chagas T, Pelc M, Goncalves PHR, Antoniazzi I, Gonzalez JW, Ayuela A, Lopes JMJ, Oliveira MH, Magalhaes-Paniago R, and Malachias A.

Carbon 142, 580-591 (2019)

Quantum dots in graphene systems are currently of interest due their electronic and optical properties and their possible use in innovative device applications. Researchers from CFM and DIPC have studied the growth of triangular nanostructures patterned on bilayer graphene films on SiC (0001) surface using hydrogen intercalation.

The authors report on triangular nanostructures using scanning tunneling microscopy and spectroscopy in collaboration with international, experimental partners. The triangular islands arise from extended stacking faults in the SiC substrate whose effects can be seen on graphene layers that are formed on top of them. Depending on local hydrogen intercalation, the spectroscopic measurements reveal distinct electronic responses that range from single- to double-layer graphene. Intermediate states were also found as a consequence of the partial hydrogen intercalation process. High-resolution topographic scanning tunneling microscopy images at resonant bias voltages inside triangular nanostructures show that the bottom layer of the bilayer graphene film is still bonded to the substrate. Therefore, within the triangular nanostructures there is a coexistence of carbon atoms bounded and unbounded to the substrate. For a better understanding of the phenomena, researchers have advanced a theoretical model using atomistic calculations. The local density of states for free standing bilayer graphene is modified locally, within the triangular, nanometer-size structures, showing confinement effects because of the strong interaction with the substrate depending on incomplete hydrogen intercalation.

These findings on triangular graphene nanostructures could be promising from the point of view of applications, as arrays with distinct electronic response are potentially interesting for high-density data storage with hidden bit capabilities.

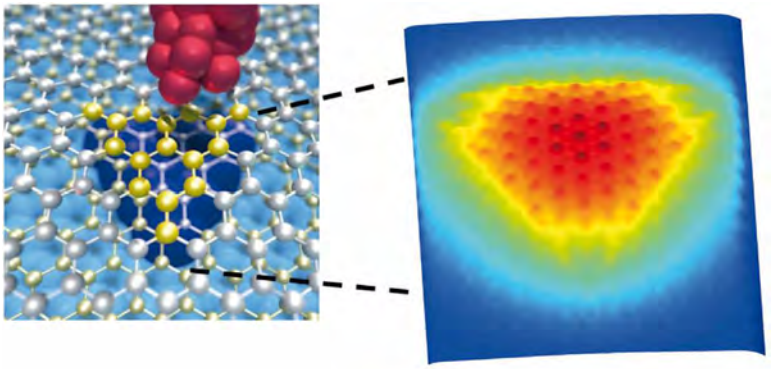


Figure: *Bilayer graphene with triangular nanostructures scanned by the STM tip. Schematic view and simulation of the STM measurement on the triangular nanostructure.*

HIGHLIGHT

Phonon collapse and second-order phase transition in thermoelectric SnSe

Aseginolaza U, Bianco R, Monacelli L, Paulatto L, Calandra M, Mauri F, Bergara A, and Errea I.

Physical Review Letters 122, 075901 (2019)

Thermoelectricity is an interesting material property that allows transforming waste heat into electricity. Good thermoelectric materials need to be good electric conductors and good thermal insulators at the same time, the so-called phonon glass and electron crystal. Due to the potential industrial applications of thermoelectric devices, a huge research effort is devoted to enhance the thermoelectric efficiency. The intrinsic single crystal of SnSe was recently found to be the most efficient thermoelectric material. In this work, Aseginolaza et al. show that very strong anharmonic effects provide its low thermal conductivity, explaining its interesting thermoelectric properties. The authors expect similar strong anharmonic effects in other good thermoelectric materials.

TAt room temperature, SnSe is a narrow gap semiconductor and at ~800 K suffers a structural phase transition to a phase with higher symmetry. In the high symmetry phase, the electronic band gap decreases while the thermal conductivity is kept very low, properties that provide high thermoelectric efficiency. Experimentally, there is discrepancy about the transition; some works claim that it is a first order transition and others that it is second order. There is also an experimental discrepancy about the thermal conductivity in the whole temperature range. As it is expected for an orthorhombic system, experiments by Ibrahim et al. show a very anisotropic thermal conductivity, with a value of ~1 W/mK (at 700 K) for measurements in the YZ plane. Experiments by Zhao et al. show almost no anisotropy and very low values for the thermal conductivity (~0.3 W/mK at 800 K).

In this work, by applying the Landau Theory of Second Order Phase Transitions and the Stochastic Self-Consistent Harmonic Approximation (SSCHA) to calculate the free energy, the authors show that the transition is second order and it is driven by the collapse of a zone border phonon mode. By making anharmonic phonon calculations within the SSCHA they show that SnSe is a strongly anharmonic material because its phonon spectrum suffers a big anharmonic correction. On top of that, they calculate the phonon spectral functions and strongly anharmonic features are present like shoulders, broad peaks and satellite peaks deviating from the typical harmonic behavior. These calculations will be crucial to understand future inelastic scattering experiments in the high symmetry phase and other materials with second-order phase transitions.

These thermal conductivity calculations in the high symmetry phase clearly show that there is anisotropy between in-plane and out-of-plane measurements and quantitatively agree with experiments by Ibrahim et al.. Therefore, Aseginolaza et al. suggest that the results by Zhao et al. may suffer from non-intrinsic effects, showing for the first time that non-perturbative anharmonicity is an critical ingredient to get a thermal conductivity in agreement with experimental evidence.

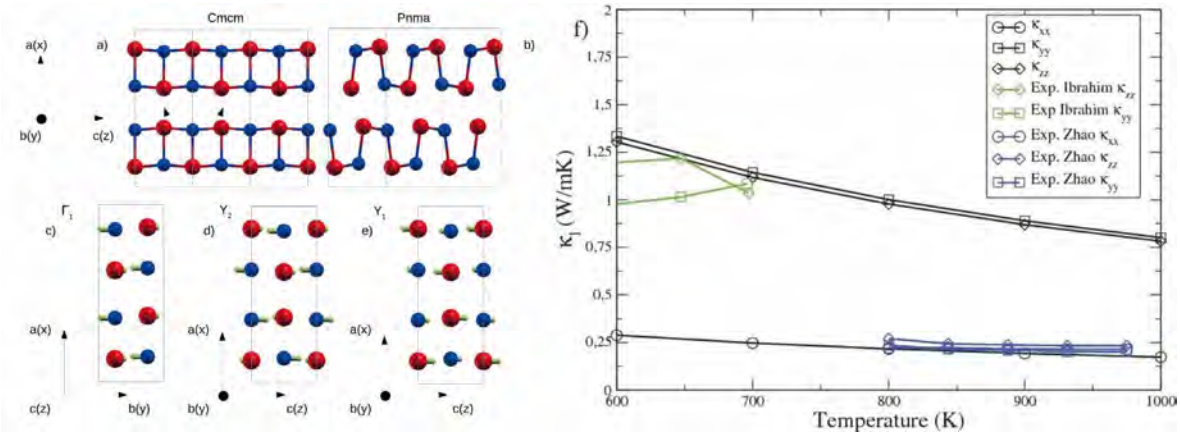


Figure (a) and (b) *show the XZ face of the high (Cmcm) and low (Pnma) symmetry phases respectively. Figure (e) shows the atomic displacements of the phonon mode that drives the transition between the two phases. Figure (c) and (d) show atomic displacements that are strongly anharmonic and show non-Lorentzian profiles in the phonon spectral function. Figure (f) shows the experimental and calculated lattice thermal conductivities. The green and blue lines correspond to experiments by Ibrahim et al. and Zhao et al. respectively. Black lines correspond to thermal conductivity calculations including anharmonicity at a non-perturbative level with SSCHA.*

HIGHLIGHT

Theory of spin Hall magnetoresistance from a microscopic perspective

Zhang XP, Bergeret FS, and Golovach VN.

Nano Letters 19, 6330 (2019)

In analogy to the ordinary Hall effect, the spin Hall effect (SHE) describes the spin-dependent deflection of electrons during transport in systems with strong spin-orbit coupling. Such a conversion of charge currents into transverse spin currents is employed now at the forefront of Spintronics to build a new generation of energy-saving electronics, exploiting the spin degree of freedom of the electron.

A manifestation of the SHE in a normal metal (NM) with spin-orbit coupling is the dependence of the magnetoresistance (MR) on the direction of the applied magnetic field when the metal is in contact with a magnetic insulator (MI), such as in NM/ MI structures. This effect, called spin Hall magneto-resistance (SMR), has been observed in several experiments as a modulation of the MR signal when the magnetization direction of the MI is changed by an external magnetic field. The origin of SMR lies in the electron's spin-dependent scattering at the NM/MI interface. Thus, by changing the mutual angle between the polarization of spin current and the MI magnetization, one is able to modulate the rate at which the electron spin relaxes.

Although the SMR theory is well established and provides a good qualitative description of the effect, it does not describe the dependence of the resistivity on the strength of the applied magnetic field B, nor on the temperature T. The interface parameters, which are at the heart of the SMR effect, have traditionally been regarded as phenomenological ones in every experiment, because their computation was thought to be a formidable task, which could only be, carried out by ab initio methods.

Originally, the SMR was observed in Pt thin films deposited on the insulating ferrimagnet $Y_3Fe_5O_{12}$ (YIG). Recent experiments explored other MIs and showed that the SMR effect depends strongly on both B and T, as well as on the magnetic state of the MI. A theory accounting for both the microscopic nature of magnetism in the MI and the spin dynamics of the conduction electrons in the NM near the interface was strongly desired.

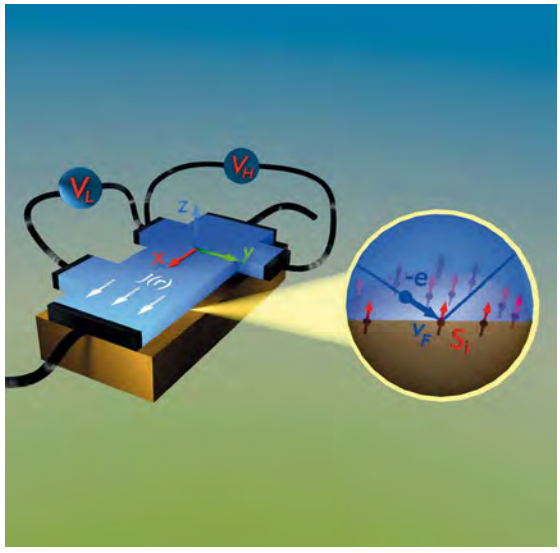


Figure: *Sketch of a Hall bar fabricated from a thin metallic film (blue) deposited on the surface of a magnetic insulator (brown). The electron scattering at the interface during which the electron spin interacts with local moments on the surface of the MI is at the heart of the SMR effect.*

> The theory presented in this work provides a tool to reveal by electric measurements the magnetic properties of interfaces

In this work, a team from the Mesoscopic Physics Group with researchers from CFM and DIPC presents a general theory of the electronic transport in NM/MI structures.

The spin-dependent scattering at the NM/MI interface is described via a microscopic model based on the exchange coupling between local moments on the MI surface and itinerant electrons in the NM. In this theory, the temperature and magnetic field dependence of the interfacial kinetic coefficients (such as spin-mixing conductance) is expressed in terms of spin–spin correlation functions in the MI.

The theory presented in this work does not only explain experiments on a variety of magnetic insulators, such as YIG, EuS, and $LaCoO_3$, but also provides a tool to reveal by MR measurements the magnetic properties of NM/MI interfaces. Furthermore, the theory predicts novel striking behaviors of the MR as a function of B-field, which can be understood in terms of an interplay between the SMR and the Hanle effects.

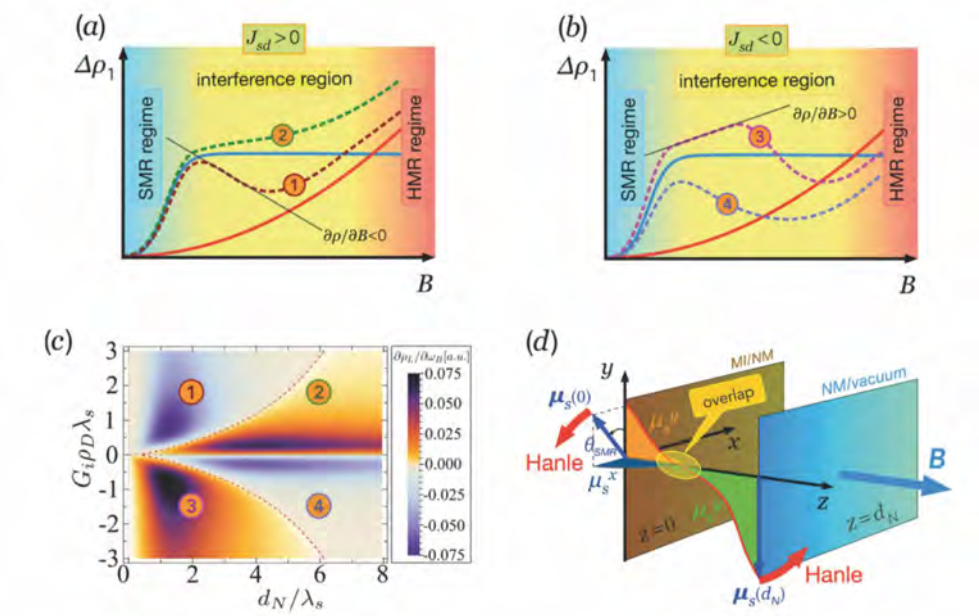


Figure: *Different behaviors of the MR predicted by the microscopic theory for a ferromagnetic (a) and antiferromagnetic (b) exchange coupling between the localized moments of the MI and the conduction electrons in the NM. (c) Separation of the parameter space (dN, Gi) into different regimes of interest, with dN being the thin-film thickness and Gi the imaginary part of the spin-mixing conductance. The regions 1–4 correspond to the four kinds of behavior shown in (a) and (b). (d) Sketch of the spin accumulation μs at the thin-film interfaces as created by the SHE and altered by the SMR and HMR effects.*

HIGHLIGHT

Multiflat Bands and Strong Correlations in Twisted Bilayer Boron Nitride: Doping-Induced Correlated Insulator and Superconductor

Xian LD, Kennes DM, Tancogne-Dejean N, Altarelli M, and Rubio A.

Nano Letters 19, 4934 (2019)

An international team of researchers has for the first time demonstrated that twisted bilayer boron nitride (TBBN) is an even more exciting novel system that turns out to be an excellent platform to realize new correlated phases and phenomena. Exploration of its electronic properties shows that in contrast to twisted bilayer graphene in twisted bilayer BN multiple families of 2,4, and 6-fold degenerate flat bands emerge without the need to fine tune close to a "magic angle". This results in dramatic and tunable changes in optical properties and exciton physics, and providing an additional platform to study strong correlations in low dimensional materials.

Twisted bilayer graphene has recently been identified as an intriguing novel system with potential high impact on fundamental as well as applied research. It is intensely debated because it could host unconventional topological superconductivity (a milestone towards the realization of universal quantum computing) as well as provide novel inroads to the long-standing problem of explaining the mechanism driving high-temperature superconductivity. The present work published in Nano Letters opens up a new route of research of phenomena linked to strongly electron correlations and new phases of matter in low dimensions considering different classes of 2D materials stacked at a twist, which the authors exemplify by performing large-scale numerical ab-initio investigations of twisted bilayer boron nitride. They find that, in contrast to twisted bilayer graphene, many multiple nearly degenerate at bands emerge for which correlations become very relevant. The results provided show that twisted bilayer boron nitride has many new key features that are highly desirable for future experiments and could open up entirely novel fields of research.

First, due to the massive nature of the Dirac Hamiltonian governing boron nitride (in contrast to the massless nature of graphene) the appearance of at bands is not limited to the so-called "magic angles" as in twisted bilayer graphene. Not having to ne-tune the angle should increase the experimental accessibility considerably while still keeping the interesting feature of promoting correlation effects intact. Secondly, in twisted bilayer boron nitride three families of two-fold, three-fold and four-fold degenerate bands emerge, thus generalizing the two-fold degenerate case of twisted bilayer graphene, and potentially allowing even more complex

band structures and thus phases of matter. The bands, with large effective masses and with charge distributions localized in specific sub-domains of the moire supercell are expected to modify the optical properties of insulating samples, in particular affecting the excitonic part of the spectrum in a drastic way. Thirdly, in doped or photo-doped samples, the authors demonstrate that the correlations at energies close to the two-fold degenerate at bands lead to physics much akin to that reported for twisted bilayer graphene. In addition, the different families of degenerate at bands can be probed in the same sample by simply varying the lying, thus expanding the novel physics discovered in graphene. This elevates twisted bilayer boron nitride to a prime candidate for future experimental studies.

The present work will spark many more experimental as well as theoretical studies in the novel realm of twisted bilayer materials, where the exploration of the possibilities of this emerging field is at its very beginning (at the crossroad of the fields of strong correlations, materials science, topology and quantum computing). The results reported here considerably broaden the viewpoint on this blossoming field of science, opening the door to similar work in other 2D twisted materials (that the authors are also pursuing).

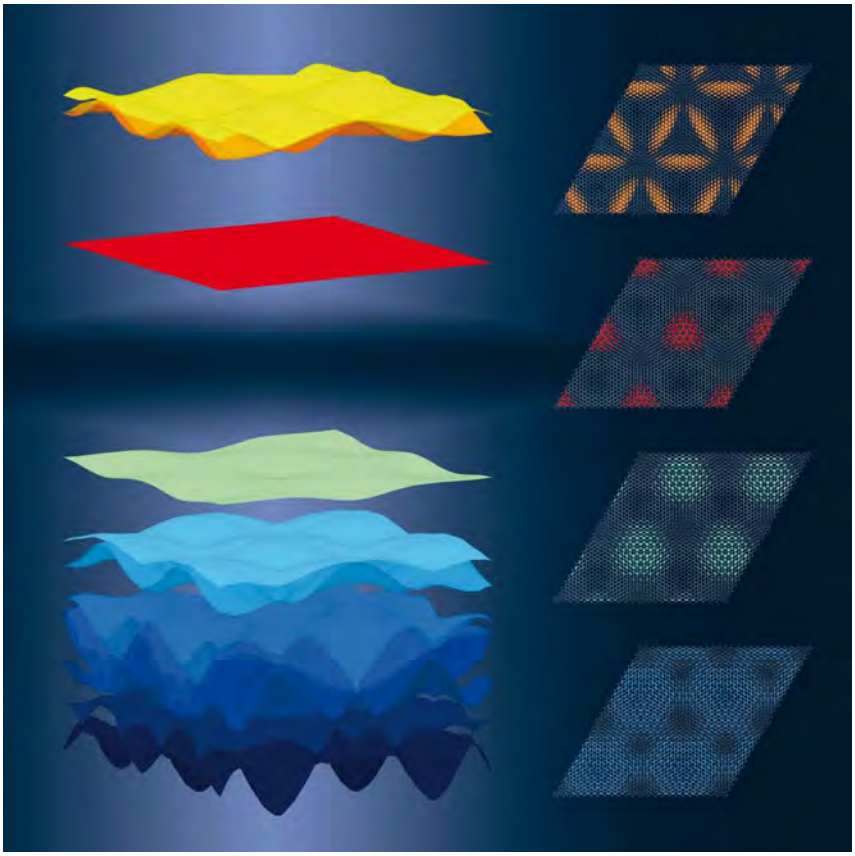


Figure: *Atomic and electronic structures of twisted bilayer BN. Schematic illustration of the possible configurations in twisted bilayer hBN that have the same Moiré pattern. Showing the localization of electronic states in the flat bands.*

HIGHLIGHT

Mechanisms and dynamics of mineral dissolution: A new kinetic Monte Carlo model

Martin P, Manzano H and Dolado JS.

Advanced Theory and Simulations 2, 1900114 (2019)

Mineral dissolution is a fundamental process in geochemistry and materials science. It is controlled by the complex interplay of atomic level mechanisms like adatoms and terraces removal, pit opening, and spontaneous vacancy creation that can be gradually activated at different energies. Though the development of a comprehensive atomistic model is key to go deeper into the understanding of this phenomenon, existing models had failed to reproduce the abrupt dependence of the dissolution rate with the Gibbs free energy (ΔG).

In this work researchers from the CFM in collaboration with researchers from Tecnalia R&I and the UPV/EHU have presented the first atomistic model capable of reproducing the experimentally observed sigmoidal dependence of the dissolution rate with the Gibbs free energy.

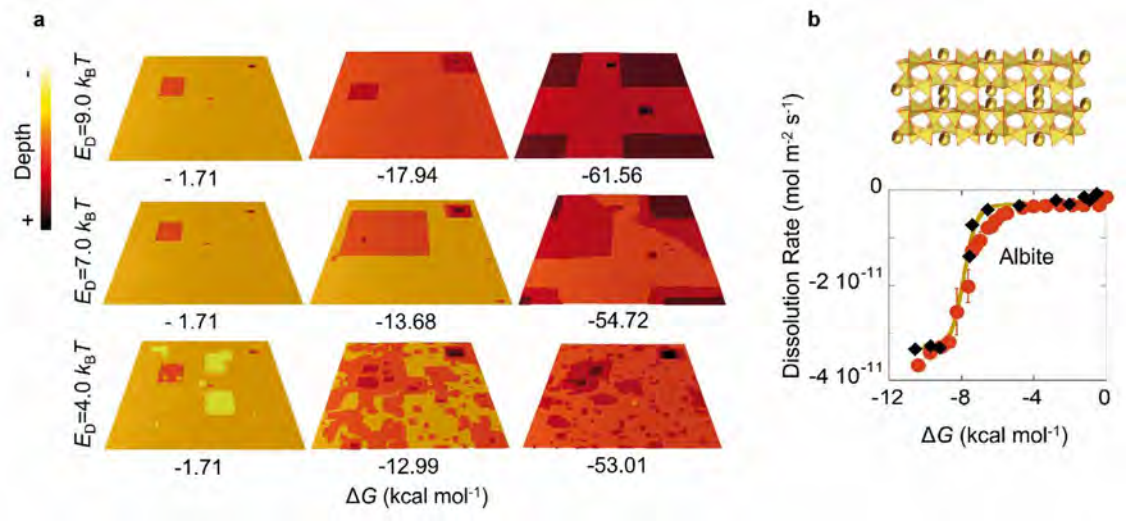


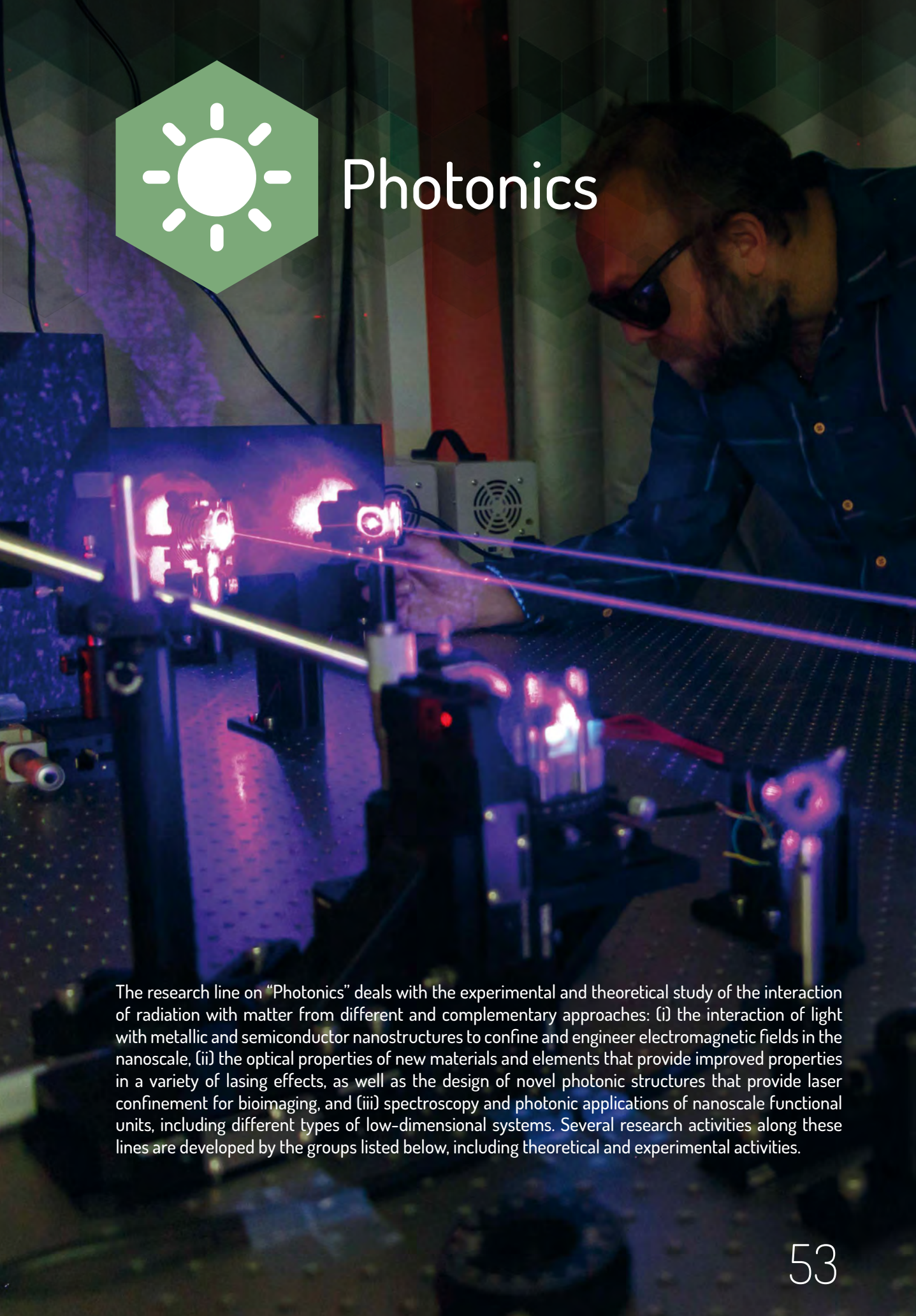
Figure (a) *Impact of the dissolution energy (E_D) on the surface dissolution patterns obtained for a Kossel crystal close at three dissolution stages: From the left to the right, close to equilibrium, at the dissolution increase onset and far away from equilibrium.* (b) *Comparison between the experimental rate of an archetypical mineral like albite (black diamonds) with the new kMC predictions (red dots) and empirical fitting schemes (brown line).*

Indeed ***Martin et al.*** calibrated their kinetic Monte Carlo (kMC) model to correctly fit the dissolution rates of several representative minerals like albite, smectite, labradorite, alite, or feldspar.

The main novelty of the new kMC model consisted in taking into account the microscopic reversibility of the chemical reactions by adding a new precipitation term to the usual Transition State Theory (TST) dissolution equation. This term turned to be crucial to successfully capture the complex dissolution phenomena. As a such, three different dissolution mechanisms naturally emerged from the simulations depending on dissolving energy and the Gibbs free energy: (i) initial irregularities dissolution at close to equilibrium conditions, (ii) pit opening and step retreat when a critical value of the Gibbs free energy is reached, and (iii) spontaneous vacancy opening at far from equilibrium conditions when the characteristic dissolution energy is low enough. The model also confirmed the generally accepted idea that the onset for the dissolution rate increase is originated by the opening of pits, which constantly supplies terraces for step retreat.

Interestingly, according to the simulations, when the dissolution and precipitation energies are sufficiently low and high respectively, there can exist close-to-equilibrium dissolution modes where spontaneous vacancies creation and pit opening can occur before adatom and terrace removal. These dissolution modes have not been previously reported, and call for experimental attention.

In summary, the work of ***Martin et al*** sheds new light on the subtle dissolution mechanisms, and can open the door to the development of a comprehensive theoretical framework for dissolution and other surface-related phenomena like etching.



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.

12 Theory of Nanophotonics

Group Leader: Javier Aizpurua Iriazabal, Research Professor, CSIC

The activity of the "Theory of Nanophotonics" group is devoted to the theoretical study of the interaction between electromagnetic radiation and nanostructured materials. The research activity of the group focuses on the theoretical study of the excitation of plasmons, quantum dots and dielectric nanostructures in the context of a variety of microscopy and spectroscopy 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.

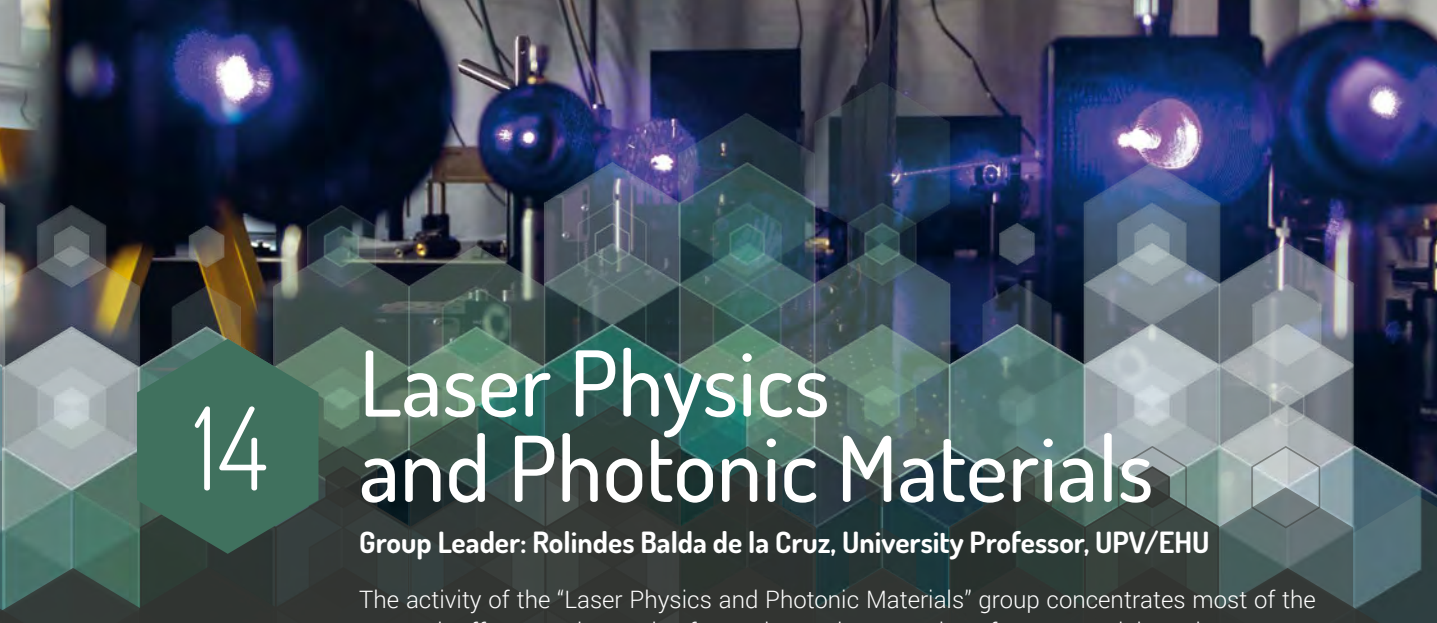
In recent years, the following specific objectives have been addressed by this group: (i) understanding and characterization of the collective excitations of the electron gas, plasmons, in a variety of spectroscopy and microscopy techniques, (ii) study of metallic nanostructures as electromagnetic field 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.

13 Nanomaterials and Spectroscopy

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

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.



14 Laser Physics and Photonic Materials

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

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.

15 Quantum Nanophotonics Laboratory

Group Leader: Gabriel Molina Terriza, Ikerbasque Professor, MPC

The Quantum Nanophotonics Laboratory is composed by a team of scientists endeavoring to unveil the physics of the interactions of quantum light and matter at the nanoscale. The group experiments with exotic states of light such as single photon states, entangled photons or squeezed states of light and force them to interact with very small structures, aiming to control the quantum features of nanoparticles by exploiting their interaction with light. This allows to design more precise quantum enhanced sensors, improve information processing and above all, pierce through the frontiers of knowledge and excite our curiosity.

The Laboratory was created in early 2018 and since then has expanded to encompass a series of experimental techniques, including optical spectroscopy with classical and quantum light, development of quantum sources of light, quantum control of nanostructures, optical tweezers and optical levitation.

Currently, the laboratory hosts three optical tables, an optically addressable closed-cycle cryostat, a set of tunable laser sources, and an optical tweezers platform, among other optical equipment.

HIGHLIGHT

Taming ultrafast electrons with light

Ludwig M, Aguirregabiria G, Ritzkowsky F, Rybka T, Marinica DC, Aizpurua J, Borisov AG, Leitenstorfer A, and Brida D.

Nature Physics. DOI: 10.1038/s41567-019-0745-8

The electric field oscillation contained in a single ultrashort laser pulse can be used to drive electron motion at sub-femtosecond time scales within a nanoscopic gap, creating a circuit that otherwise would be open. A combined theoretical and experimental study of this ultrafast electron motion allows for tracing the photocurrent induced in the nanogap, clarifying the interplay between the carrier-envelope phase of the driving pulse, the plasmonic resonance and the electrons quiver motion.

The technological achievements in electronics have been remarkable over the course of the last decades with a major impact to the society that has drastically evolved towards the digital age. The fundamental principle behind this revolution is quite simple: the capability to open and close an electrical circuit as fast as possible in order to perform operation on a sequence of bits. In fact, modern electronic transistors can operate at frequencies well beyond 1 GHz, corresponding to 1 billion operations per second. However, the standard technological platform for obtaining these results is based on semiconductors like Silicon and has reached a bottleneck with objective difficulties in improving the speed at which electronic components work.

To overcome this limitation, an international collaboration involving researchers of the Theory of Nanophotonics Group at CFM and DIPC, in Donostia / San Sebastian, together with the theoretical group of Andrei Borisov at the Institute of Molecular Sciences of Orsay (France), teamed up with the experimental groups of Alfred Leitenstorfer at the University of Konstanz (Germany), and Daniele Brida at the University of Luxembourg, to exploit short light pulses as a means to control the ultrafast motion of electrons in a metallic nanocircuit (see figure 1). Since light has the advantage that it oscillates at frequencies that are a million times higher than the ones achieved by electronic circuits, the capability to control an electronic circuit at optical frequencies opens up a roadmap able to revolutionize fast data processing and computing in the future. While this goal is still far

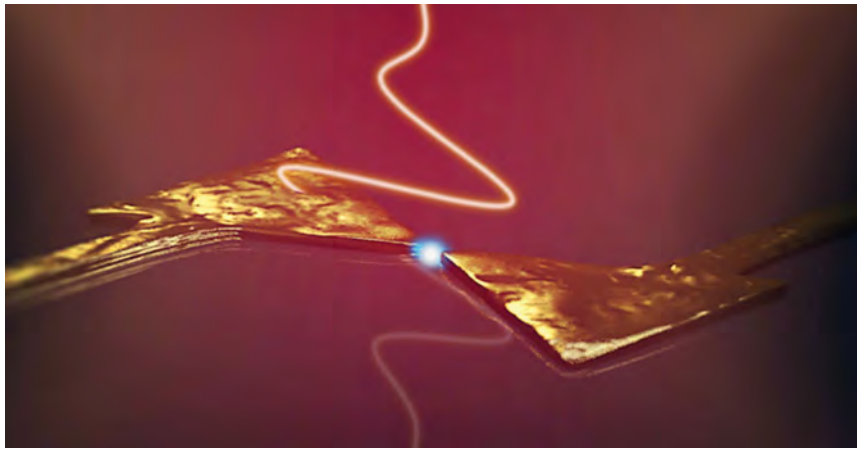


Figure 1: *Bowtie nanoantenna (bright areas) forming a nanogap (blue bright spot). An incident single-cycle laser pulse generates ultrafast motion of electrons within the cavity, which are able to close the electrical circuit.*

from being completely achieved, the experiments and theoretical development performed in this study by the international team, allows for tracing the electrons motion at the ultrafast times driven by the taming photon pulse (see figure 2).

This work provides a detailed description of the experiments and theoretical modeling, which serves to understand how electrons move within this open gap between two metallic nanostructures, and thus, on how light interacts with matter especially in a regime where it is possible to observe quantum phenomena at temporal and spatial scales that were previously inaccessible. The impact of this study has also broader applications to nanotechnology, particularly in optoelectronics, since special nanodevices with high structural precision are being fabricated to manipulate the electrons in the experiments, as well as in laser science, thanks to the development of novel laser sources able to deliver extremely short pulses at high repetition rate, enabling more complex non-linear operations in optoelectronic nanocircuits.

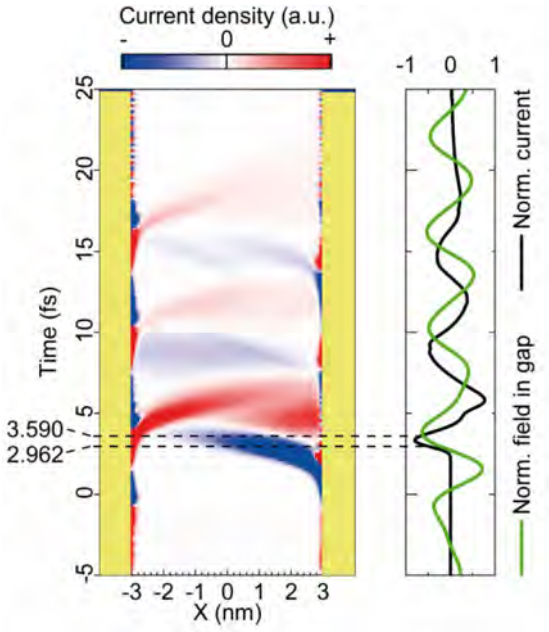


Figure 2: *Evolution in time of the current density of photoelectrons in a metallic nanogap driven by an ultrafast optical pulse, which generates an induced field in the gap (green line on the right hand side). The total normalized current is shown with a black line to the right.*

HIGHLIGHT

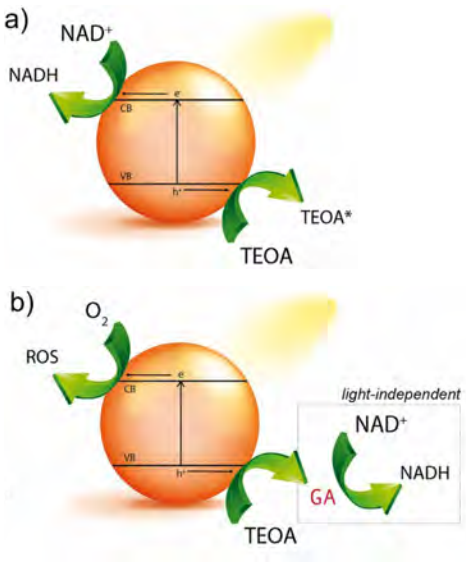
Photocatalytic cofactor regeneration involving triethanolamine revisited: The critical role of glycolaldehyde

Kinastowska K, Liu J, Tobin JM, Rakovich Y, Vilela F, Xu ZT, Bartkowiak W, and Grzelczak M.

Applied Catalysis B-Environmental 243, 686 (2019)

The need for efficient conversion of light into useful fuel pushes researchers to find innovative approaches to produce solar fuel. The photo-regeneration of cofactor molecules, using photocatalysts is a cost-efficient strategy of producing added-value chemicals since cofactor can be implemented in many enzymatic reactions.

The difficulty in photoregeneration of cofactor molecule remains in the need of using another molecule - sacrificial electron donor- that donates electron(s) to photoexcited photocatalyst to be later passed to the acceptor (NAD+) (Figure 1a). Although water is the target electron donor, it is a chemically stable molecule, requiring the use of alternative solutions. One of such alternatives is triethanolamine (TEOA) that has become a flagship electron donor in research labs since its first implementation in the late seventies. Although its electron-donating character has been demonstrated, little is known on the exact degradation pathway, especially in the process of cofactor regeneration.



A team of researchers, including Ikerbasque researchers Yury Rakovich (CFM & DIPC) and CSIC researcher Marek Grzelczak (CFM & DIPC), shows that triethanolamine can decompose to glycolaldehyde, an intermediated product that is able of reducing NAD+ to NADH, regardless the presence of light (Figure 1b).

These findings show that in the presence of oxygen the degradation of triethanolamine and regeneration of cofactors molecules are not necessarily coupled processes, as has been though for many years. They showed that in the presence of any photocatalyst (conjugated microporous polymer, carbon nitride, platinum nanoparticles and titanium dioxide) and light TEAO decomposes to glycolaldehyde, which induces NADH regeneration in the dark, even after the photocatalyst is removed.

Apart from obtaining a better picture of cofactor regeneration, these basic-research results came with exciting perspectives for future works. It turns out that glycolaldehyde (the simples form of sugar) is of high value in the field of prebiotic chemistry. Glycolaldehyde is an essential intermediate in formose reaction, a process that involves the self-accelerated synthesis of biologically relevant sugars from formaldehyde as a starting material.

Figure: *Schematic illustrating reduction of NAD+ to NADH*

HIGHLIGHT

Site-selective symmetries of Eu^{3+}-doped $BaTiO_3$ ceramics: a structural elucidation by optical spectroscopy

Serna-Gallen P, Beltran-Mir H, Cordoncillo E, West AR, Balda R, and Fernandez J.

Journal of Materials Chemistry C 7, 13976 (2019)

The crystallographic nature and spectroscopic properties of non-equivalent europium sites in $BaTiO_3$ have been investigated. Time-resolved fluorescence line narrowing (TRFLN) spectroscopic results are consistent with the preference of Eu^{3+} to occupy Ba^{2+} sites regardless of the nominal compositions and target substitution mechanism. However, TRFLN results also showed that the dopant could also occupy Ti^{4+} sites, highlighting the amphoteric character of Eu^{3+}. The existence of non-equivalent europium sites with different spectroscopic properties could have an impact on the optical properties of doped-$BaTiO_3$ ceramics and device applications.

Barium titanate, $BaTiO_3$, has been a longstanding material for electronic devices due to its broad spectrum of properties, such as spontaneous polarization, high dielectric permittivity in the paraelectric phase and piezoelectric response. Luminescent trivalent lanthanide ions (Ln^{3+}) incorporated into solids have been greatly studied not only because of their application in emission displays and lasers but also for their ability to change and tune material properties depending on the site occupation of Ln^{3+} in the host lattice. Elucidating the distribution of Ln^{3+} involves determining if it occupies a single site (Ba^{2+} or Ti^{4+}) or multiple sites (both Ba^{2+} and Ti^{4+}), the solubility limit in each site, and how this distribution changes with lanthanide concentration

This collaborative work carried out by the groups led by Eloísa Cordoncillo (University Jaume I, Castellón) and Rolindes Balda (CFM, UPV/EHU), gives a plausible elucidation of Eu^{3+} site occupation in micron-sized $BaTiO_3$ ceramics prepared by sol-gel synthesis based on the nominal compositions $(Ba_{1-3x}Eu_{2x})TiO_3$ and $Ba(Ti_{1-x}Eu_x)O_{3-x/2}$, where two possible substitution mechanisms are addressed. Time-resolved fluorescence line narrowing (TRFLN) shows the presence of five different crystal field sites for europium ions and possible symmetries are inferred for each one. The solubility limit of the lanthanide ion was found to be about 3 mol%. The experimental results are consistent with the preference of Eu^{3+} to occupy Ba^{2+} sites regardless of the nominal compositions and target substitution mechanism. However, TRFLN results reported that the dopant could also occupy Ti^{4+} sites, highlighting the amphoteric character of Eu^{3+}. The existence of anti-Stokes and Stokes vibronic sidebands in the $^5D_0$ $^7F_{0,1}$ transitions of Eu^{3+} ions is confirmed. This can explain the lack of resolution found in room temperature spectra of these transitions due to vibronic mixing of the excited levels. The presence of non-equivalent europium sites with different spectroscopic properties could have a decisive impact not only on the optical properties of doped-$BaTiO_3$ ceramics but also on their wide range of device applications.

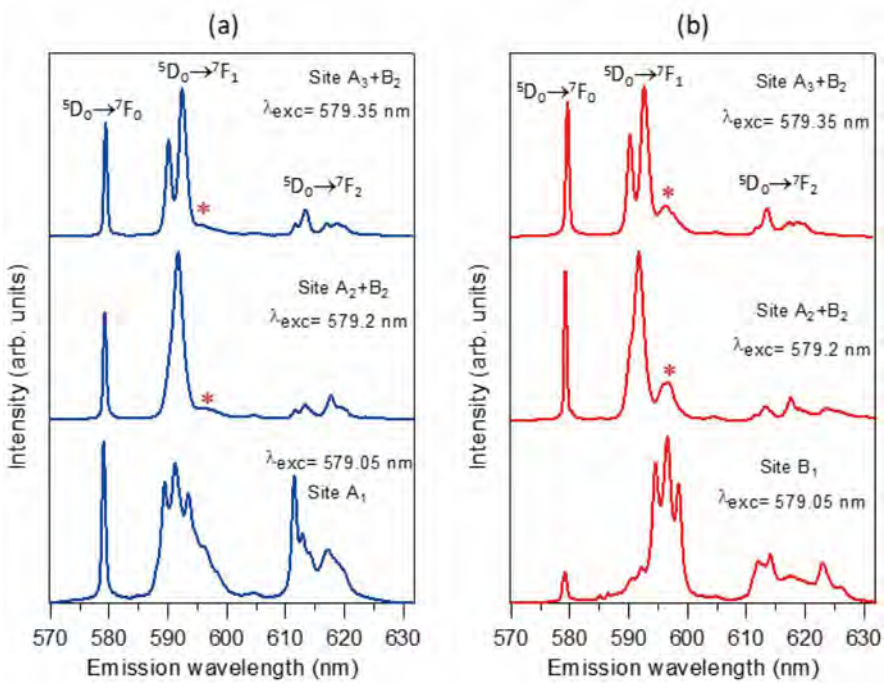


Figure: Low temperature (10 K) TRFLN $^5D_0 \rightarrow {}^7F_{0\text{-}2}$ emission spectra of samples (a) 3%-Ba and (b) 3%-Ti showing the emissions from sites A_1, A_2, A_3, B_1, and B_2 (red stars). The abbreviations A_i and B_i refer to Eu^{3+} occupying Ba^{2+} and Ti^{4+} sites, respectively.

Table: Description of the different crystal field sites for Eu^{3+} ion in doped-$BaTiO_3$ samples. The abbreviations Ai and Bi refer to Eu^{3+} occupying Ba^{2+} and Ti^{4+} sites, respectively.

λ_{exc} (nm)	Site	Symmetry
579.05	A_1	Low (near particle surface)
	B_1	Low (near particle surface)
579.20	A_2	Close to cubic
	B_2	Cubic (*Oh*)
579.35 [a]	A_3	Trigonal (C_{3v} or C_3)

[a] The emission of Site B_2 can also be observed when pumping at 579.35 nm due to vibronic coupling.

HIGHLIGHT

Unfolding the colored centers in nanodiamonds

Roberts RP, Juan ML, and Molina-Terriza G.

Physical Review B 99, 174307 (2019)

Diamond is one of the most extraordinary materials on Earth. Its mechanical, electrical and optical properties make it suitable for many technologies. The color of diamond is given by defects on the atomic structure which can be manufactured and behave as "artificial atoms". In this work, the authors experimentally study the Nitrogen Vacancy center, which has important applications in quantum technologies.

The Nitrogen Vacancy (NV) center in diamond is one of the best know quantum emitters that can be found in diamond. It can be present in both the bulk form of diamond or in nanodiamonds, making it suitable for applications in nanotechnology. It can be used as a biological marker, as diamond is inert and biocompatible. As a quantum emitter, it has been proposed as a potential source of quantum light for quantum communications. In addition, the long coherence of its electronic states makes it ideal as a magnetic quantum sensor. Therefore, the potential of NV centers to become a transformative technology is enormous.

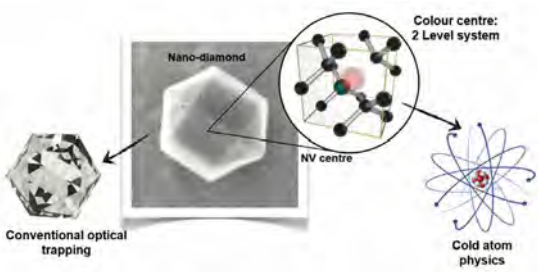


Figure 1: *Nanodiamonds have a crystalline structure of Carbon atoms. Often, this structure contains defects, such as the Nitrogen Vacancy center, which can act as "artificial atoms" which are held in the crystalline structure. These defects can emit light in the same way as normal atoms do.*

Nevertheless, one main drawback of the use of NV centers is that the two-level system model for the electronic transitions is only valid in very simple experimental conditions. On the other hand, the dynamics of the electronic states when pumped with different laser frequencies become rather complex. This complexity is enhanced because many of the transition mechanisms are not fully understood. In this experimental work, Roberts et al. perform a series of fluorescence measurements, including different pump wavelengths and external magnetic fields. In this way, they have been able to experimentally fit the different possible physical mechanisms of electronic transitions in the NV.

The main result is that the charge state interconversion, i.e. the NV capturing and releasing an electron, going from a negatively charged state to a neutral one, is responsible for the infrared quenching of the fluorescence of the center. Interestingly, this effect depends on the spin state of the negatively charged state. This has implications for the spin polarization of the NV and has to be taken into account in magnetic sensing applications.

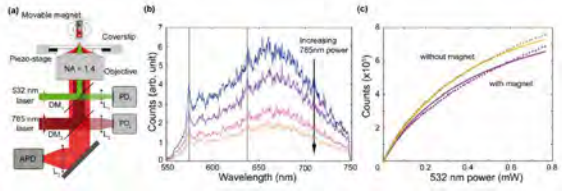


Figure 2: *(a) Set-up of the experiment. The nanodiamond is illuminated with different light sources and its emission is collected with an avalanche photo diode (APD) (b) Depletion of the emission of the nanodiamond when more near infra-red light is used (785nm) (c) The emission is affected by magnetic fields, which indicates that the spin dynamics of the NV center plays a central role in the photodynamics.*

Polymers and Soft Matter

16 Polymers and Soft Matter

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

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) single-chain-nano-particles and related systems; (iii) applying methods and concepts of polymer physics to the study of proteins; (iv) glass-transition phenomena in nano-structured polymer glasses; (v) unveiling polymer dynamics at intermediate length scales by combining coherent neutron scattering and MD-simulations; (vi) exploiting atomistic MD-simulations to unravel structural and dynamical properties in different aqueous systems; (vii) cyclic polymers with control of dipolar microstructure. 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.

At the end of 2019, Prof. Ikerbasque Félix Fernández Alonso joined this line to reinforce research on the use of neutron techniques for materials characterization.

HIGHLIGHT 1

Mesoscale Dynamics in Melts of Single-Chain Polymeric Nano-Particles

Arbe A, Rubio-Cervilla J, Alegria A, Moreno AJ, Pomposo JA, Robles-Hernandez B, de Molina PM, Fouquet P, Juranyi F, and Colmenero J.

Macromolecules **52**, 6935 (2019)

Single-Chain Nano-Particles (SCNPs) are soft nano-objects halfway between linear chains and 'standard' nano-particles. Studies of systems based on SCNPs allows to look on the still scarcely explored interface between the soft matter fields of polymers and colloids. Here Arbe et al. have addressed the fundamental question of the impact of purely intra-molecular cross-linking on the properties of a polymer melt.

Single-Chain Nano-Particles (SCNPs) are obtained by intra-molecular cross-linking of individual macromolecular chains. The unique properties of a melt exclusively composed by SCNPs have been here addressed by a concerted effort, combining advanced chemistry and a battery of different experimental tools, including `macroscopic' (calorimetry, dielectric and mechanical spectroscopy) and `microscopic' (neutron diffraction and neutron spin echo, NSE) techniques.

Neutron scattering techniques, providing spatial resolution through the scattering vector (Q) dependence of the measured magnitudes, have been applied to per-deuterated systems, to follow collective features. The comparison with a bulk sample composed by the long linear counterpart chains (precursor macromolecules without internal crosslinks) demonstrates that the structure and dynamics at local length scales including the inter-chain distances (in particular, the structural relaxation) are hardly sensitive to intra-molecular cross-links (see Figs. 1 and 2). The authors were also able to extend their neutron experiments to the so far almost virgin territory of the so-called intermediate length scales (ILS). The ILS region corresponds to length scales larger than the typical inter-molecular (for small molecules) or inter-chain (for polymeric objects) distances but not yet in the hydrodynamic regime. At ILS, a pronounced slowdown of the collective dynamics is observed (Fig. 2), associated to emerging structural heterogeneities with a characteristic length of about 1 nm (Fig. 1). On the other hand, the dielectric relaxation spectra reveal an enhanced intensity in the frequency region below the α-process loss peak –signature of an additional mechanism for relaxation--, and rheological experiments show a strong impact on the rubbery plateau properties.

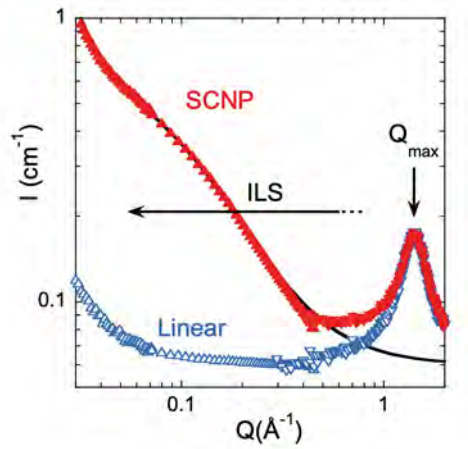


Figure 1: *Differential cross section of the bulk sample consisting of linear precursor chains (blue) and of SCNPs (red symbols) obtained by SANS. The vertical arrow shows the position of the inter-chain peak Q_{max}.*

This combined study allowed the authors to propose a new picture. Local globulation and compartmentalization into domains composed by internal loops induced by the intra-molecular cross-links has three main impacts: (i) introducing heterogeneities with nanometer length scale; (ii) increasing the complexity of the dynamics; in particular, a new relevant relaxation mechanism appears, presumably associated to the internal domains; and (iii) strongly modifying the entanglement network of the macromolecules.

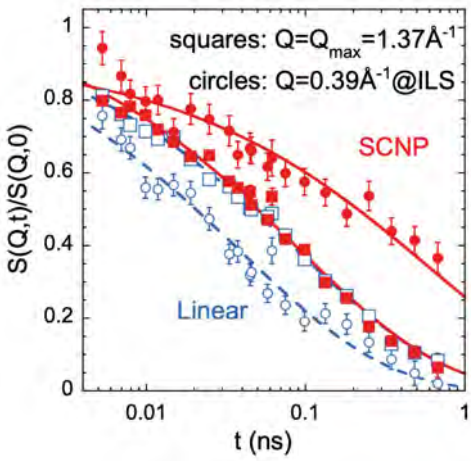


Figure 2: *Normalized dynamic structure factor measured by NSE at Q_{max} (probing the α-process) and a representative Q-value in the ILS region. Lines are fits to stretched exponential functions.*

HIGHLIGHT 2

Revealing the time-dependent tube dilation in entangled polymer blends with neutron spin echo combined with dielectric spectroscopy and rheology

Malo de Molina P, Alegría A, Allgaier J, Kruteva M, Hoffmann I, Prévost S, Monkenbusch M, Richter D, Arbe A, and Colmenero J.

Physical Review Letters 123,187802 (2019)

An open question on the dynamics of entangled polymers is how the topological constraints are released by mobile neighboring chains or, in other words, how the constraining tube is dilated. This work by members of the Polymers & Soft Matter group (in collaboration with Forschungszentrum Jülich, Germany and Institut Laue-Langevin, France) reports the direct microscopic observation of the time-dependent tube dilation in iso-frictional blends.

Polymeric materials are ubiquitous in every-day life. Their mechanical performance, industrial processing and other end-use properties are determined by their dynamics. Hence, it is important to fundamentally understand how the macromolecules move in the material, in particular in modern materials with increased complexity.

Nowadays, it is well accepted that the viscoelastic properties of high molecular weight polymer melts are controlled by entanglements: topological constraints imposed by mutually interpenetrating and uncrossable polymer chains. In the tube model for entangled chains, these constraints are represented by a fictitious tube that restricts the lateral motion of the polymer chain within its diameter leading to a reptation motion of the chain along the tube.

However, the pure reptation model fails in real materials, which are polydisperse and most of the times multicomponent. In these cases other mechanisms compete with reptation, mainly, contour length fluctuations (CLF)—fluctuations of the length of the tube—and constraint release (CR) — probe relaxation driven by the motions of surrounding chains. CR becomes particularly important in polydisperse melts and binary blends, especially where long polymer chains are mixed with short additives of the same chemistry (iso-frictional blends) but sometimes of different polymer architecture. A simplified model of the many-body CR mechanism, called dynamic tube dilation (DTD), considers that CR leads to an increase with time of the tube diameter. The effective terminal tube dilation of the long chains in polymer blends can be determined by obtaining the long-time tube diameter from macroscopic techniques such as dielectric spectroscopy and rheology. However, these techniques cannot resolve the time evolution of the tube dilation. This work exploits the spatial and time resolution of neutron spin echo to directly probe the time-dependent tube dilation in model blends based on polyisoprene with different topologies. By combining NSE with rheology and dielectric spectroscopy, the characteristic time that governs tube dilation is identified as the terminal time of the additive. This finding will help elucidate the mechanism for constraint release and, thus, will facilitate the design of polymeric materials with the desired rheological properties.

> This work exploits the spatial and time resolution of neutron spin echo to directly probe the time-dependent tube dilation

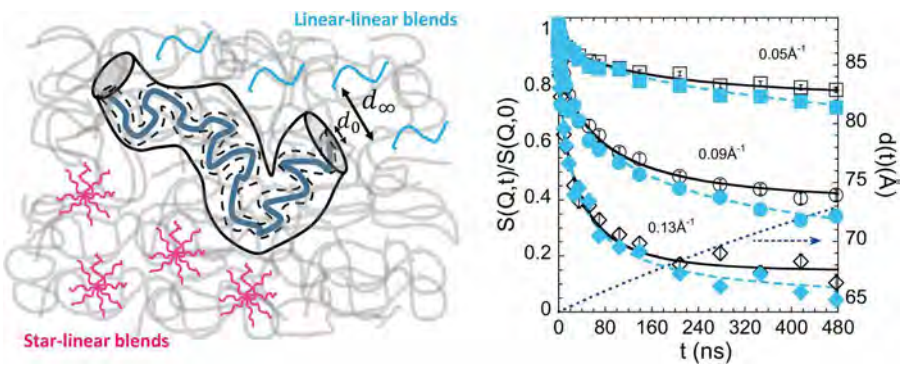


Figure: *Left: Schematic representation of the tube dilation in linear-linear and star-linear blends. Right: Time evolution of the chain dynamic structure factor measured by NSE for the long chains in the pure matrix (black) and in the blends with short linear polymer (blue). The dotted line shows the increase of the tube diameter in the blend as the time increases.*

HIGHLIGHT 3

Glassy dynamics of an all-Polymer nanocomposite based on polystyrene single-chain nanoparticles

Robles-Hernandez B, Monnier X, Pomposo JA, Gonzalez-Burgos M, Cangialosi D, and Alegria A.

Macromolecules **52**, 6868 (2019)

Robles-Hernandez et al. investigate the glassy dynamics of an all-polymer nanocomposite, made of a linear polymer, poly(vinyl methyl ether (PVME)), with dispersed single-chain nanoparticles (SCNPs) based on polystyrene (PS), by combining broadband dielectric spectroscopy (BDS) and fast scanning calorimetry (FSC). These results highlight the hybrid nature of this kind of materials, intermediate in between that of a conventional polymer nanocomposite and that of a miscible polymer blend.

Formulation of polymeric composites is a very useful approach to tune material properties starting from already existing materials. Usual polymer nanocomposites contain inorganic fillers with a tendency to segregate. A new alternative is obtaining all-polymer nanocomposites by mixing conventional linear polymer chains with SCNPs generated by intramolecular collapse of single linear chains of a different polymer. In these systems, the SCNPs can be deformed/penetrated affecting the dynamics and thermodynamics of the matrix. A question that remains to be answered in particular, is how the molecular dynamics and the equilibrium recovery in this new kind of nanocomposite compares with that observed in more conventional nanocomposites prepared using inorganic hard nanofillers.

In this work, the authors have addressed this question by investigating the glassy dynamics around the glass transition of a mixture of the linear PVME with 10% wt PS-based SCNPs. By BDS, they characterize the molecular motions of PVME segments in the system with negligible contributions from the SCNPs. By FSC, which is sensitive to both components of the mixture, accessing both the time scale of the molecular motions responsible for the glass-transition phenomenon, the so-called α-relaxation, and the kinetics of equilibrium recovery of the system during physical aging. The results obtained for the mixture PVME/SCNPs are also compared with those corresponding to an equivalent mixture of PVME with the linear polymer precursor (Prec) of the SCNPs. This set of data allowed identifying the major peculiarities of this all-polymer nanocomposite as compared to more conventional nanocomposites.

The major results are summarized as follows: i) the segmental dynamics of the matrix is not much influenced by the presence of SCNPs (Figure 1). ii) However, BDS makes evident the presence of a slow component of the segmental dynamics of the mixture that would be related with the PVME in intimate contact with the SCNPs (Figure 2). iii) The final equilibrium recovery of the all-polymer nanocomposite involves extremely large time scales (a factor of 100) as compared with the equivalent blend of linear chains. iv).

The present results suggest that the nanocomposite picture can be depicted as approximately consisting of 87% pure PVME matrix with inclusions of PVME penetrated PS-SCNPs (25/75 wt%).

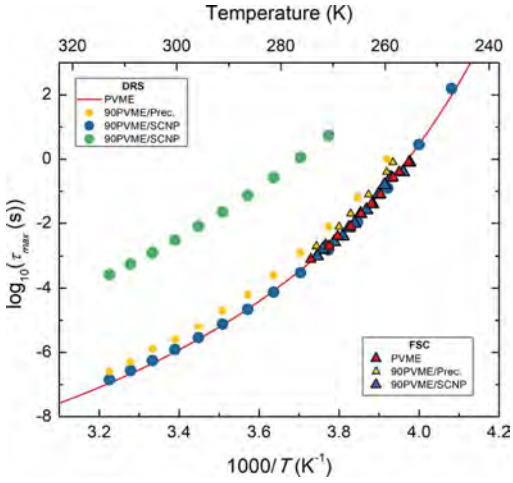


Figure 1: *Temperature dependence of the relaxation time for the 90PVME/SCNP sample obtained by BDS (blue and green circles) and by FSC (blue triangles); and for 90PVME/Prec blend obained by BDS (yellow circles) and by FSC (yellow triangles). The solid line corresponds to a description of the data of pure PVME.*

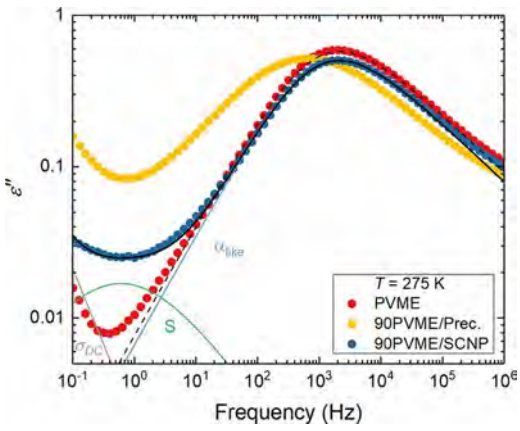


Figure 2: *Dielectric losses of PVME (red), 90PVME/Prec (yellow), and 90PVME/SCNP (blue). The dashed line is the fitting curve corresponding to the α-relaxation of pure PVME. The solid black line is the fitting curve obtained by the addition of α-relaxation (blue), an additional slow mode (green), and DC contribution (gray) in the 90PVME/SCNP sample.*

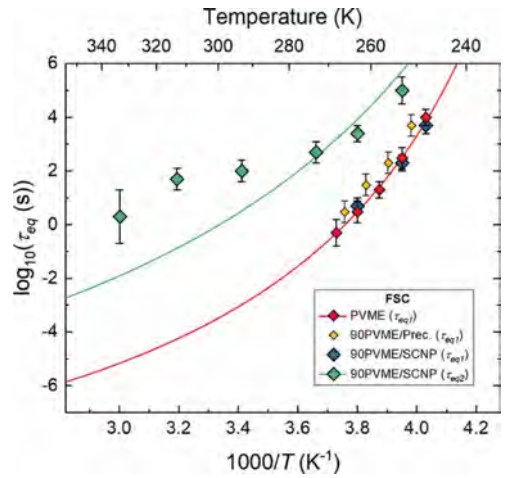


Figure 3: *Temperature dependence of the characteristic equilibration time obtained by FSC, for neat PVME (red, τeq1), 90PVME/Prec (yellow), and 90PVME/SCNP (blue and green, respectively). The red solid line is the fit of pure PVME. The green solid line is traced by vertically shifting the red solid line according to the BDS results.*

Colloquium: Atomic spin chains on surfaces

Choi DJ, Lorente N, Wiebe J, von Bergmann K, Otte AF, and Heinrich AJ.

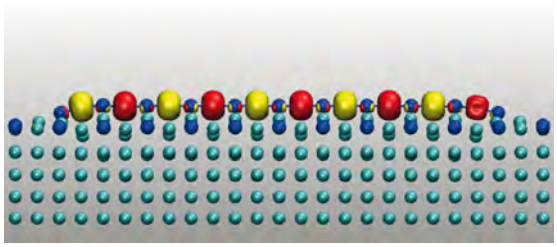
Reviews of Modern Physics 91, 041001 (2019)

An open-shell atom has a spin that can be oriented in the presence of an external magnetic field giving rise to a magnetic moment. When there are several spins, their mutual interaction can orient them, and gives rise to the rich field of magnetism. The simplest systems one can think of are lines of atoms. These one-dimensional systems are called spin chains and they are incredibly difficult and complex. The best theories and intricate calculations have been devoted to unravelling their physics and exploring all possibilities. Experimentally, a lot of attention has been devoted to their construction and analysis.

The progress in local probe techniques has allowed researchers to study matter atom-by-atom. Single atom manipulation has been achieved, allowing positioning them on solid surfaces, and creating new systems. Spin chains are natural systems to study with local probes. This article explores the work recently done, showing the different ingredients at play in the rich physics of this fully quantum objects.

The article explores the physics of spin chains on surfaces, reviewing the theory and addressing the particular concepts that are needed to understand these objects. The article proceeds with a review of experiments following the different substrates where the spin chains are going to be hosted. Contrary to having self-standing spins, the present work on surfaces needs to take into account and assess the effect of the surface. Indeed, the article shows that regarding the type of coupling between the spin chain and the host, the physics can varied very much, from having exotic correlated systems like spinors, to usual magnetic excitations like spin waves, and also Haldane gaps or Majorana bound states on superconducting surfaces.

The article is a vivid account of on-going research that should have an impact in the design of future magnetic systems as well as experiments with the new local probes that are being currently tested such as electron-spin resonance with the scanning tunneling microscope. All this shows the excitement of the field and the very complex physics that can be nowadays studied by looking at single atoms in atomic systems.



A chain of open-shell atoms (Mn_9) on a CuN surface on top of a Cu substrate. Cu is not magnetic, and the nitrogen on the first layers allows to have a directional Mn structure grown on it. The last atom on the right side of the chain is an Fe atom. The N atoms of the surface are promoted between the Mn atoms to glue the spin chain together. The colors display the orientation of the local magnetic moments (red is up and yellow is down) showing that the spin chain is antiferromagnetically oriented. This system behaves like an object with a spin of ½ despite the fact that each local spin is either 2 (Fe) or 5/2 (Mn) showing how different the outcome can be from the individual constituents of the spin chain.

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 CHEMICAL-PHYSICS LAB

The "Surface Chemistry" laboratory is equipped with an Ultra High Vacuum chamber combining different surface characterization techniques: X-Ray Photoemission Spectroscopy (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.)
- Sub- and super-critical reactors (Novoclave 600ml HP 500bar/500°C)
- An isothermal calorimeter (TAM Air 8-channel model from TA Instruments) for cements characterization.

PHOTONICS

LASER SPECTROSCOPY LAB

In the "Laser Spectroscopy" laboratory, continuous and time-resolved (with nano-picoseconds excitation laser sources) spectroscopy systems 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) microscopy setup (MicroTime200, PicoQuant) with single molecule detection sensitivity, equipped with two lasers (405 and 485 nm), two single-photon counting avalanche photodetectors, heating stage, and cryostat. The system contains the complete optics and electronics for recording all main aspects of the luminescence dynamics down to single nanoparticle/ molecule level with wide range of capabilities: 2D and 3D Confocal photoluminescence microscopy imaging o Single molecule imaging; 2D and 3D Fluorescence Lifetime Imaging (FLIM); the minor carriers lifetime mapping; carriers recombination dynamics; and Forster Resonance Energy Transfer (FRET).

Other available set-ups include:

- QUEPRO high-performance spectrophotometer connected to IX71 Olympus microscope for microphotoluminescence spectroscopy
- MayaPro2000 spectrophotometer (Ocean Optics)
- Cary50 spectrophotometer (Agilent) for absorption and transmission spectroscopy
- Cary 3500 (Agilent) with kinetics and temperature control
- 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
- Thermal cycler (Applied Biosystems) for 96 wells
- Two programmable syringe pumps (WPI) operating at wide range of flow rates
- Two illumination sources of 150 W quartz halogen fiber optic illuminator (Dolan-Jenner) equipped with the set of bandpass and long-pass filter (Edmund Optics, and Intor)

- Portable photometer equipped with global radiometer sensor (400 – 2000 nm)
- Oxygen sensor (Neo Fox, Ocean Optics)
- Thermocouples operating in wide range of temperatures and solvents (Thorlabs).

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 mm x 1800 mm 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); an 808nm, 10mW, diode (from Thorlabs)
- A source of entangled photons based on a periodically poled potassium titanyl phosphate (ppKTP) crystal
- 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 materials 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 + Light scattering Wyatt miniDAWN TREOS, viscosimeter ViscoStar II and Optilab rEX Refractive Index Detector
- Nanoparticle size and z-potential meter: Malvern Zetasizer Nano
- Viscometers: 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 CHARACTERIZATION LAB

- The "Thermal Characterization" 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)

RHEOLOGICAL CHARACTERIZATION LAB

The "Rheological 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

ABSORPTION SPECTROSCOPY TECHNIQUES LAB

The "Absorption Spectroscopy Techniques" 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 structural 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 120 TFLOPS of Theoretical Peak Performance, and a computing time of about 36 000 000 computing process unit (CPU) hours per year (about 4100 computing cores). It consists of three 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 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 file system, 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 each node, giving a total of 1088 cores and about 1.1TB of memory.
- *Ekhi* cluster, designed specifically for novel Quantum ESPRESSO calculations, is composed of 28 computing nodes with two Xeon Cascade Lake-SP 6230 processors (40 computing cores) and 96GB of memory on each node, with an InfiniBand FDR interconnection network, giving a total of 1120 cores and 2.7TB of memory.

These three HPC clusters give service to a variety of computational needs in the center, mainly related to ab-initio calculation of advanced materials, which is a transverse working topic at CFM. Apart from these clusters, 11 workstations are devoted to run specific numerical applications as well as to data analysis, code development and testing.

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:

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 (180-700K) 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 (100-800K) 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.

HIGH PERFORMACE COMPUTING (HPC) SUPPORT

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

RESEARCH OUTPUT

Among all the articles published at CFM, **79 %** were published in the framework of **international collaborations**, showing the international dimension and positioning of the Centre in the field of Materials Science.

ISI Publications
199 in 2019

Q1 Publications
138 in 2019

D1 Publications
61 in 2019

H-Index
125

ISI Web of Science citations
11289*

*As of March 2020 (according to Publons)

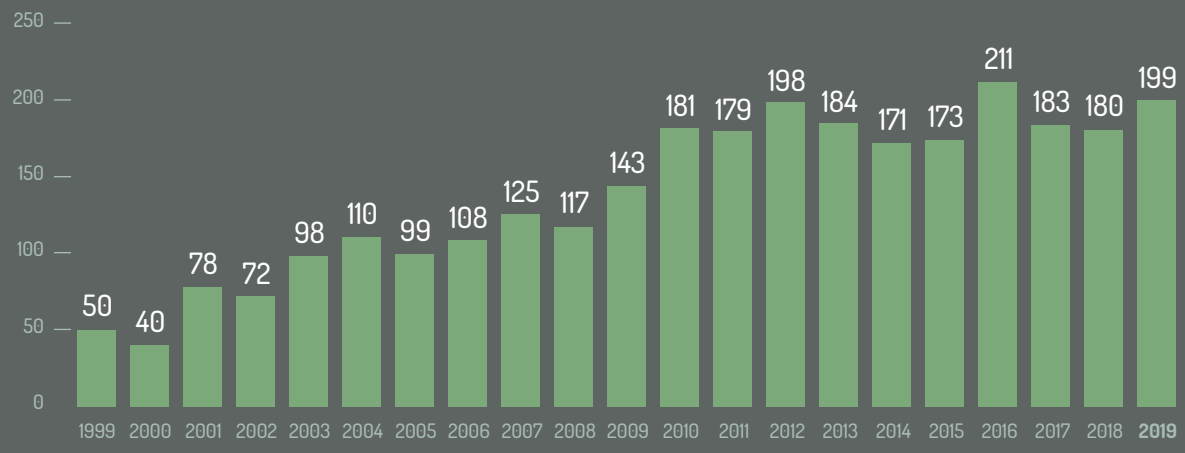
Average impact factor of the center
6.35 in 2019

RESEARCH OUTPUT

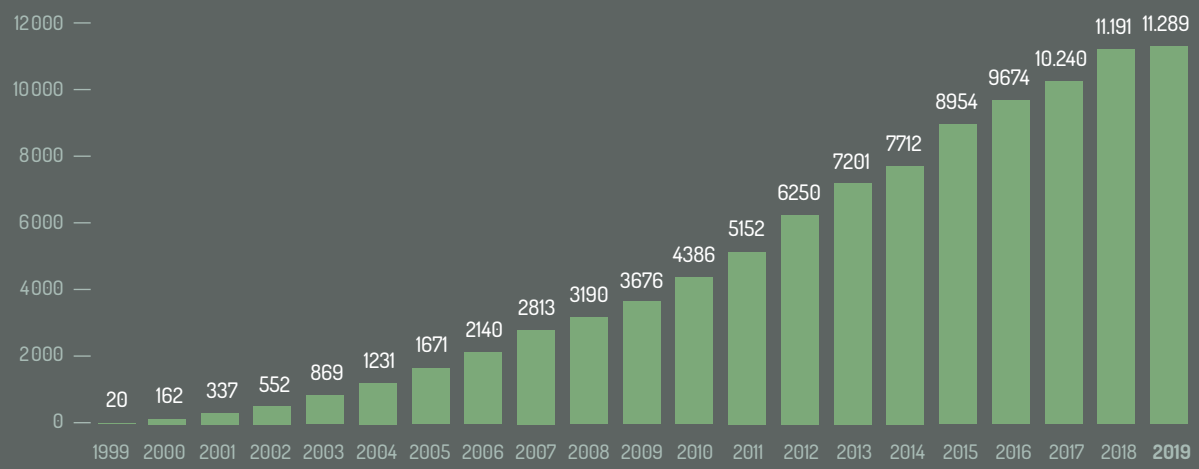
	2010	2011	2012	2013	2014	2015	2016	2017	2018	**2019**
ISI PUBLICATIONS	181	179	198	184	171	173	211	184	178	**199**
Q1	134	144	149	139	131	129	178	116	105	**138**
D1	-	-	-	-	52	50	74	59	63	**61**

Source: Web of Science Core collection and InCItes Journal Citations Report. The values of Q1 and D1 correspond to those calculated according to the anual citations report published the previous year. In 2016 and 2017, the journal Physical Review B dropped from Q1 to Q2. This fact explains the inconsistent low Q1 values observed in the years 2017 and 2018. In 2018 Physical Review B was Q1 again.

PUBLICATIONS



CITATIONS



Total number of ISI citations since 1999: 102.064
H index (March 2020): 125

Total number of publications with impact factor larger or equal than that of Carbon (7.47):

Journal	Number of articles	Impact factor
Chemical Reviews	1	54.30
Nature	1	43.07
Science	1	41.06
Nature Materials	1	38.88
Reviews of Modern Physics	1	38.29
Nature Physics	1	20.11
Advanced Functional Materials	1	15.62
Journal of the American Chemical Society	2	14.69
Applied Catalysis B-Environmental	1	14.22
ACS Nano	4	13.90
Nano Letters	6	12.27
Angewandte Chemie-International Edition	1	12.26
Nature Communications	5	11.88
Small	1	10.86
Physical Review Letters	9	9.23
NPJ Computational Materials	1	9.20
Laser & Photonics Reviews	1	9.06
Progress in Surface Science	1	8.76
Carbon	2	7.47

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8 **Boosting and balancing electron and hole mobility in single- and bilayer WSe2 devices via tailored molecular functionalization**
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Merino-Dez N, Paz AP, Li JC, Vilas-Varela M, Lawrence J, Mohammed MSG, Berdonces-Layunta A, Barragan A, Pascual JI, Lobo-Checa J, Pea D, and de Oteyza DG.
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BOOK CHAPTERS

Single-chain polymer nanoparticles: Synthesis, characterization, simulations and applications

Wiley-VCH / John Wiley & Sons
Editor: Jose A. Pomposo

Advances in quantum chemistry- Chapter six - Collective electronic excitations on the $MgB_2(0001)$ surfaces

Elsevier
Vyacheslav M. Silkin, Evgenii V. Chulkov, and Pedro M. Echenique

Polymer colloids: Formation, characterization and applications – Glass transition and crystallization in colloidal polymer nanoparticles

Royal Society of Chemistry (RSC)
Daniele Cangialosi

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 programs through the Department of Material Physics of UPV/EHU, as well as setting complementary training activities devoted to 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.

TRAINING ACTIVITIES

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. 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, currently 61 pre-doctoral researchers 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.

DEFENDED PhD THESES

- **New Synthetic Routes, Topologies and Physical Properties of Single-Chain Nanoparticles**
  Author: Thomas Gambino
  Supervisors: José A. Pomposo
  Group: Polymers and Soft Matter
  03/04/2019

- **Theory of Ultrafast Charge Transfer from Localized Quantum States at Surfaces**
  Author: Moritz Müller
  Supervisors: Daniel Sánchez Portal
  Group: Modelisation and Simulation
  05/04/2019

- **Theoretical Description of Low-Energy Excitations in Nanostructures as Probed by Fast Electrons**
  Author: Andrea Konečná
  Supervisors: Javier Aizpurua and Rainer Hillenbrand (CIC nanoGUNE)
  Group: Theory of Nanophotonics
  17/05/2019

- **Understanding of Plasticizer Effect on the Temperature Dependence of Mechanical and Dielectric Relaxation Function of Polymers of Interest for Tire Formulation**
  Author: Jon Rubio
  Supervisors: Ángel Alegría and Juan Colmenero
  Group: Polymers and Soft Matter
  04/06/2019

- **Magneto-Optical Characterization of Magnetic Thin Films and Interface Structures**
  Author: Patricia Riego Saavedra
  Supervisors: Andreas Berger (CIC nanoGUNE) and Jose María Pitarke
  Group: Quantum Theory of Materials
  15/07/2019

- **Magnetic Properties of Co on Different Environments**
  Author: Iker Gallardo
  Supervisors: Andrés Arnau and Fernando Delgado (Universidad de La Laguna, Tenerife)
  Group: Modelisation and Simulation
  04/11/2019

- **On-Surface Synthesis and Electronic Structure Characterization of Graphene Nanoribbons**
  Author: Nestor Merino
  Supervisors: Dimas García de Oteyza and Nacho Pascual (CIC nanoGUNE)
  Group: Dimas García de Oteyza's group at CFM
  12/11/2019

- **Transport and Spectral Properties of Low-Dimensional Superconductors in the Presence of Spin-Dependent Fields**
  Author: Julie Baumard
  Supervisors: Sebastián Bergeret and Alexander Bouzdin (Université de Bordeaux)
  Group: Mesoscopic Physics
  19/12/2019

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 pre-doctoral researchers. This year, 13 pre-doctoral researchers spent 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 2019:

- **Antton Babaze**
  Institut des Sciences Moleculaires d'Orsay, ISMO (France)
  4 March - 4 June

- **Oscar Rodriguez**
  Chemistry Department in the Pennsylvania State University (USA)
  2 May - 29 July

- **Maud Formanek**
  Universitá di Roma "La Sapienza" (Italy)
  16 June - 20 July

- **Carlos Escudero**
  Chalmers University of Technology, Goteborg (Sweden)
  1 August - 1 November

- **Julen de la Cuesta**
  University of Oslo - UiO (Norway)
  1 September - 30 November

- **Cristina Mier**
  Institute Physical and Chemistry Materials Strasbourg (France)
  1 September - 31 November

- **Carmen Gonzalez**
  Sincrotrón ALBA, Barcelona (Spain)
  15 September - 15 December

- **Joseba Goikoetxea**
  Peter Grünberg Institut, Jülich (Germany)
  30 September - 29 November

- **Raul Guerrero**
  Technical University of Dresden (Germany)
  1 October - 15 December

- **Jon Lasa**
  University of Vienna (Austria)
  20 October - 20 December

- **Miguel Ángel Jiménez**
  University of Zurich (Germany)
  1 October - 30 November

- **Marina Peña**
  Universidad de Alicante (Spain)
  7 October - 7 December

- **Valentina Musumecci**
  University of California (USA)
  16 November - 22 December

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, students choose to develop their 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.

THESES OF THE NANOSCIENCE MASTER SUCCESSFULLY DEFENDED IN 2019

- **Terahertz Time Domain Spectroscopy of Diabolo Antennas**
  Author: Katarina Rovenska
  Supervisor: Rainer Hillenbrand (CIC nanoGUNE)

- **Influence of Magnetic Metal-Phthalocyanine Thin Films on the Optoelectronic Properties of Single Layer Transition Metal Dichalcogenides**
  Author: Jose Manuel Pereira
  Supervisors: Reyes Calvo (CIC nanoGUNE)

- **Photoactivated Folding of Individual PVC Chains to Single-Chain Nanoparticles**
  Author: Agustín Blazquez
  Supervisors: José A. Pomposo and Ester Verde (CFM)

- **Calibration of the Atomic Layer Injection System (ALI)**
  Author: Afia O. Akyaw
  Supervisors: Celia Rogero and Sara Barja (CFM)

- **Orientation Dependence of Dynamic Phase Transitions in Highly Anisotropic Ferromagnets**
  Author: Mikel Quintana
  Supervisor: Andreas Berger (CIC nanoGUNE)

- **Boosting Nanoporous Graphene Reactivity by Chemical Doping**
  Author: Sara Lois
  Supervisors: Aran G. Lekue (DIPC)

OTHER MASTER THESES SUPERVISED BY CFM STAFF AND SUCCESSFULLY DEFENDED IN 2019

- **Laser Induced Femtochemistry on Metal Surfaces**
  Author: Maxime Infuso
  Supervisors: Maite Alducin and Iñaki Juaristi

- **Análisis Térmico y Reológico de los Cambios Producidos en Manzanas Mediante la Acción de la Poligalacturonasa**
  Author: Javier Martinez Sabando
  Supervisors: Silvina Cerveny and Juan Carlos Arboleya

- **Characterization of Noise in Interferometric Measurements**
  Author: Florian Lochon
  Supervisors: Gabriel Molina

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 are also offered the possibility to be trained in-situ at CFM, with the opportunity to interact with top quality research groups for a short stay or to fulfill their End of Course Project during the academic year. In 2019, CFM hosted the training of ten undergraduate students. Out of them, four students defended their End of Course Project during 2019.

END OF COURSE PROJECTS DEFENDED

- **Estudio de la Pilarización del Óxido de Grafito con Diaminas y la Intercalación del Polioxido de Etileno**
  Author: Maitane Romatet
  Supervisor: Fabienne Barroso and Ángel Alegría
  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 Unimoleculares Potencialmente Catalíticas a partir de Polibutadieno**
  Author: Leire Orbegozo
  Supervisor: José A. Pomposo
  Group: Polymers and Soft Matter

- **Surface Characterization of oxide surfaces on Ru(0001)**
  Author: Ane Telleria
  Supervisor: Celia Rogero, Andrés Arnau, and Sara Barja
  Group: Nanophysics Lab

UNDERGRADUATE INTERNSHIPS

CFM also offers the possibility to receive support for this training through different grant programs. In 2019 two students were granted:

- **Ninon Möhl**
  Supervisor: Lucia Vitali
  Group: Spectroscopy at Atomic Scale

- **Jon Ruiz Tarango**
  Supervisors: Silvia Arrese-Igor and Angel Alegría
  Group: Polymers and Soft Matter

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).

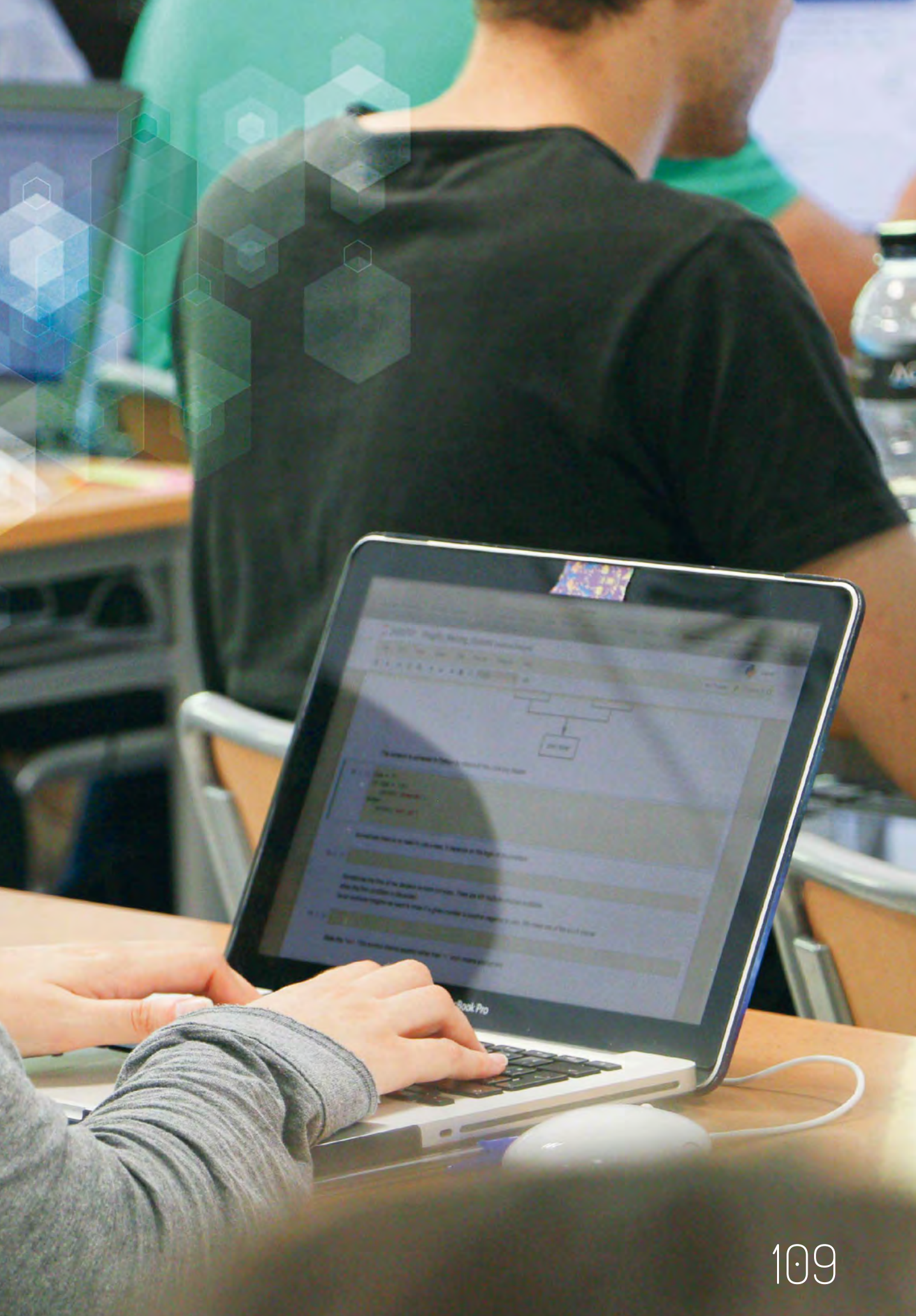
Other specialized courses about specific experimental techniques are also organized. Furthermore, a laboratory course on dielectric spectroscopy is successfully organized by CFM researcher Prof. Ángel Alegría, in which 15-20 graduate students and researchers take part yearly.

WORKSHOPS, CONFERENCES AND SEMINARS

CFM scientists have organized or co-organized several international workshops and conferences during 2019. 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.

The list of conferences, courses, workshops and seminars organized or co-organized by CFM researchers during 2019 follows:



INTERNATIONAL CONFERENCES

Symposium on Surface Science (3S`19)

Ane Sarasola, Daniel Sánchez Portal, Enrique Ortega, Andrés Arnau and Pedro Echenique
Hotel Tuc Blanc, Baqueira Beret, Spain
10-16/03/2019

10th International Meeting on Atomic and Molecular Physics and Chemistry 2019

Sergio Díaz (***Universidad Autónoma de Madrid***), Daniel J. Arismendi (DIPC-CFM), and Cristina Sanz (Universidad Autónoma de Madrid)
City Center Campus CSIC, Madrid
11-14/06/2019

Quantum Designer Physics

Daniel Loss (University of Basel, Switzerland), Francisco Guinea (IMDEA, Madrid and University of Manchester, UK), Andrés Arnau (CFM, DIPC and UPV/EHU) and Vitaly Golovach (CFM and DIPC)
Miramar Royal Palace, Donostia / San Sebastián, Spain
1-4/07/2019

Science of Cement and Related Complex Materials

Andrés Ayuela (CFM and DIPC), Jorge Sánchez Dolado (CFM and DIPC), Silvina Cerveny (CFM and DIPC), Juan José Gaitero (TECNALIA R&I), Edurne Erkizia (TECNALIA R&I), Jose Ramón Leiza (TECNALIA R&I) and Hegoi Manzano (TECNALIA R&I).
Miramar Royal Palace, Donostia / San Sebastián, Spain
15-18/07/2019

Photo and ElectroCatalysis at the Atomic Scale (PECAS 2019)

Sara Barja (Ikerbasque, CFM and DIPC, Chair), Celia Rogero (CFM), Olaf Magnussen (Kiel University), and Doris Grumelli (MPI-FKF, INIFTA - CONICET)
Miramar Royal Palace, Donostia / San Sebastián, Spain
27-30/08/2019

Frontiers of Condensed Matter

Sebastián Bergeret (CFM and DIPC), Julia Meyer (***Université Grenoble Alpes***, France), Tjerk Oosterkamp (Leiden Institute of Physics, Netherlands) and Jörg Schmalian (KIT Germany)
Les Houches, Grenoble, France
16-27/09/2019

Trends in Nanotechnology 2019

Antonio Correia (Phantoms Foundation, Spain) – Chairperson, Daniel Sánchez Portal (CFM-CSIC / DIPC) – Co-Chairperson, Massimo De Vittorio (IIT / Center for Biomolecular Nanotechnologies, Italy) Pedro Echenique (DIPC - UPV/EHU), Uzi Landman (Georgia Tech, USA), Juan José Saenz (DIPC, Spain), Josep Samitier (Institute for Bioengineering of Catalonia - ***Universitat de Barcelona***, Spain), Frank Scheffold (University of Fribourg, Switzerland), Pedro A. Serena (ICMM/CSIC, Spain), and Didier Tonneau (CNRS-CINaM, France)
Cámara de Gipuzkoa, Donostia / San Sebastián, Spain
30 September- 4 October, 2019

WORKSHOPS

Introduction to Version Control with Git

Instructor-Iñigo Aldazabal (Centro de Física de Materiales CSIC-UPV/EHU); helpers Guillermo Boyra (AZTI-Tecnalia), and Abel Carreras (Donostia International Physics Center - DIPC)
AZTI-Tecnalia, Pasajes, Spain
04/06/2019

Machine Learning in Condensed Matter Physics

Maia G. Vergniory (DIPC and Ikerbasque), Fernando de Juan (DIPC and Ikerbasque), Reyes Calvo (CIC nanoGUNE and Ikerbasque), Adolfo G. Grushin (Grenoble, France) and Iñigo Aldazabal (CFM)
DIPC, Donostia / San Sebastián, Spain
26-28/08/2019

SUPERTED 2019 Meeting (open workshop)

Celia Rogero and Sebastián Bergeret
CFM
16-17/09/2019

Jornadas TIC CSIC

Clara Cala (SGAI), Alejandro Morales (***Instituto Andaluz de Ciencias de la Tierra*** - IACT), Sonia de Diego (***Centro Nacional de Biotecnología*** - CNB), Luis Torres (***Estación Biológica de Doñana*** - EBD), Íñigo Aldazabal (***Centro de Física de Materiales*** CSIC-UPV/EHU), Guillermo Rodríguez (***Instituto de la Grasa*** - IG), Maríam Dobón (***Delegación Institucional en la Comunidad Valenciana*** - DICV), Pedro Pemau (***Centro de Biología Molecular Severo Ochoa*** - CBMSO), José M. García (***Instituto Pirenaico de Ecología*** - IPE), and Rafael Álvarez (***Centro de Investigaciones Científicas Isla de la Cartuja*** - cicCartuja).
Abades Nevada Palace, Granada, Spain
25-27/11/2019

Software Carpentry

Instructors: Iñigo Aldazabal, Emilio Ambite, Alfonso Nuñez, and Bryan Zaldivar | Helpers: Andrés Díaz-Gil, Eduardo de Cordoba, Marcos Ramírez, and Nadir Samos.
Instituto de Ciencias Matemáticas - ICMAT, Madrid, Spain
November 28, 29 and December 4, 2019

COURSES

9th Laboratory Course on Dielectric Spectroscopy

Ángel Alegría, Silvia Arrese-Igor, Danielle Cangialosi, Silvina Cerveny, and Gustavo Ariel Schwartz (CFM, DIPC, and UPV/EHU Vice-rectorate of the campus of Gipuzkoa)
CFM
27-31/05/2019

Concrete Technology – State of the Art and Future

Jorge Sánchez Dolado
Nanjing, China
21-25/08/2019

PhD SEMINAR SERIES

Since 2013, a regular series of seminars delivered by PhD students is organized at CFM. This activity continued during 2019. Approximately every two weeks, from September to June, two PhD students present updated results of their respective theses work to the whole 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 PhD seminars given in 2019 follows:

- **Heptacene on Ag(001): Synthesis and Exploration of Charging Features**
  Mohammed Sabri Gamal Mohammed
  06/02/2019

- **Surface-enhanced Molecular Electron Energy Loss Spectroscopy**
  Andrea Konečná
  06/02/2019

- **Introduction and Theory on STM Electron Spin Resonance**
  Jose Reina
  27/02/2019

- **Second-Harmonic Generation due to Plasmon-Molecule Interaction**
  Antton Babaze
  27/02/2019

- **Spectral Properties and Quantum Phase Transitions in Superconducting Junctions with a Ferromagnetic Link**
  Mikel Rouco
  20/03/2019

- **Theory of Spin Hall Magnetoresistance from a Microscopic Perspective**
  Xianpeng Zhang
  20/03/2019

- **Quasiparticles under the Electron-Phonon Interaction: A Combined Numerical and Complex-Analytical Approach**
  Jon Lafuente
  10/04/2019

- **Ab-initio study of the Electron-Phonon Interaction of a Single Fe Adatom on the MgO/Ag(100) Surface**
  Haritz Garai
  10/04/2019

- **(Classical and Quantum) Scattering of Helical States of Light**
  Álvaro Nodar
  02/05/2019

- **Tuning the Surface State of Au(111) and Cu(111)**
  Iker Gallardo
  02/05/2019

- **Calculation of Exciton Binding Energies Using TDDFT**
  Mikel Arruabarrena
  22/05/2019

- **CO Oxidation on Pt at Operando Conditions: An Approach Using Curved Crystals and Photoemission**
  Fernando García
  22/05/2019

- **Local Anomalous Hall Conductivity in Non-Collinear Spin Textures**
  Miguel Ángel Jiménez
  12/06/2019

- **Supermagnonic Domain Wall Dynamics in Layered Antiferromagnets**
  Ricardo Rama
  12/06/2019

- **5-Armchair Graphene Nanoribbons: Semiconductor, Topological, Magnetic... Something Else?**
  Alejandro Berdonces
  20/11/2019

- **Benchmarking the Starting Points of The GW Approximation for Open-Shell Molecules: A First-Principles Study**
  Masoud Mansouri
  20/11/2019

- **Anharmonic Effects in The Out-of-Plane Acoustic Vibrations of Graphene**
  Unai Aseguinolaza
  18/12/2019

- **Phonon-Polaritons In Hexagonal Boron Nitride Probed by Fast Electrons**
  Carlos Maciel
  18/12/2019

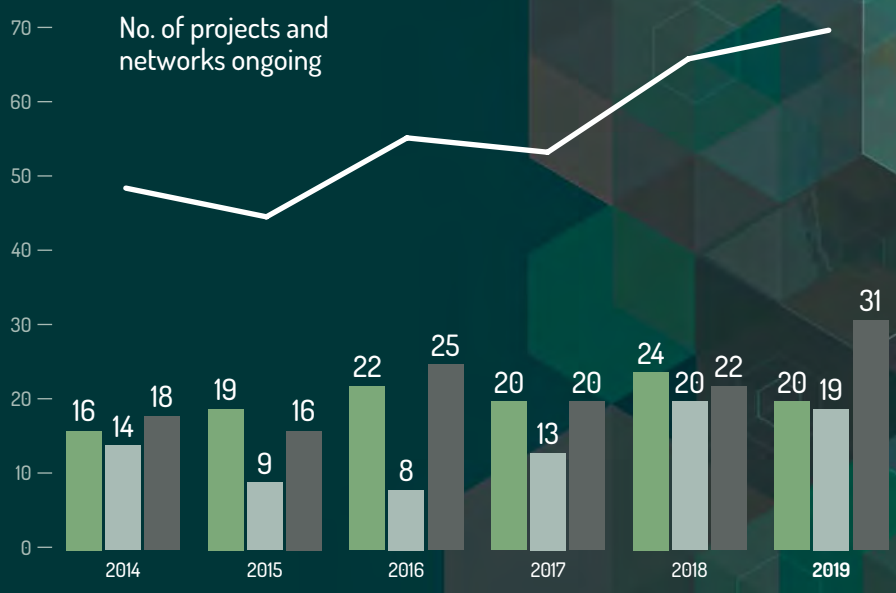
MORE SEMINARS HELD AT CFM

- **Vacuum Technologies Seminar**
  Alessandro Abatecola, Solutions Manager in Agilent Technologies
  21/03/2019

- **Charge Transfer and Transport Processes in Molecule-Substrate Systems: A Theoretical Perspective**
  Pedro Braña, Department of Physical and Analytical Chemistry, University of Oviedo
  06/05/2019

COMPETITIVE FUNDING FOR RESEARCH PROJECTS

RESEARCH PROJECTS AND NETWORKS	Competitive public fundraising in 2019
BASQUE	1 500 969 €
SPANISH MINISTRY	1 260 972 €
EUROPEAN AND INTERNATIONAL	2 054 621 €
MPC-BERC	1 224 640 €
TOTAL	**6 041 202 €**



The projects and networks that were ongoing during 2019 (a total of 70 projects/networks) are listed below according to the source of competitive funding.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BASQUE RESEARCH PROJECTS AND NETWORKS

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

- **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

- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1246-19**
  Grupo de Fisicoquímica de Superficies y Nanoestructuras
  PI: Joseba Iñaki Juaristi Oliden

- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1255-19**
  Nanophyscis Lab San Sebastián: desde la ciencia de superficies a los dispositivos
  PI: Enrique Ortega Conejero

- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1164-19**
  Q-NANOFOT-Nanofotónica cuántica para la caracterización de nuevos procesos y aplicaciones en espectroscopías moleculares, microscopía de campo cercano y tecnologías cuánticas con fotones
  PI: Javier Aizpurua Irizabal
  Co-PI: Nerea Zabala Unzalu

- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1175-19**
  PSMG - Polymers & Soft Matter
  PI: Juan Colmenero de León

- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1249-19**
  FunTheMaS - Fundamental Theoretical Materials Science
  Co-PI: Ángel Rubio Secades

- **EJ/GV, EKIZIEN 2018: Adquisición Equipamiento Científico, EC19-27**
  Recycling Preparative SEC/GPC
  PI: José A. Pomposo Alonso

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2018 RED2018, 2018-CIEN-000025-01**
  INTERFACES – Interfaces de aislantes topológicos
  PI: Lucia Vitali

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2018 RED2018, 2018-CIEN-000036-01**
  Fuente de plasma para crecimiento de nuevos materiales funcionales en condiciones de ultra alto vacío
  PI: Sara Barja Martínez

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa Coopera 2018, 2018 IZEN-000013**
  ELLAS INVESTIGAN IV: afrikar emakumezko ikertzaile batek egonaldi bat egin dezan MPCn / ELLAS INVESTIGAN IV: estancia de investigación en el MPC de una investigadora africana

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa Coopera 2019, 2019-IZEN-02**
  ELLAS INVESTIGAN V: afrikar emakumezko ikertzaile batek egonaldi bat egin dezan MPCn / ELLAS INVESTIGAN V: estancia de investigación en el MPC de una investigadora africana

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2019 RED2019, 2019-CIEN-000003-01**
  Desarrollo de nanopartículas poliméricas unimoleculares conteniendo metales divalentes como catalizadores para la síntesis de aditivos usados en la preparación de biodiesel
  PI: José A. Pomposo Alonso

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2019 RED2019, 2019-CIEN-000050-01**
  Síntesis química de materiales nanoestructurados para salud y energía
  PI: Yury Rakovich

- **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

BASQUE RESEARCH PROJECTS AND NETWORKS

- **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

- **UPV/EHU, Ikerketa Taldeak / Grupos de Investigación UPV/EHU 2018, GIU18/85**

  Desarrollo de nuevas metodologías en problemas destacados de Física de la Materia Condensada

  Partners: Aitor Bergara Jauregi and Ion Errea Lope

SPANISH MINISTRY RESEARCH PROJECTS AND NETWORKS

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

- **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 Díez Muiño
  Co-PI: Maite Alducin Ochoa

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

- **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

- **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

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

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

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

SPANISH MINISTRY RESEARCH PROJECTS AND NETWORKS

- **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

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

- **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: Sebastián Bergeret Sbarbaro
  Co-PI: Dario Bercioux (DIPC)

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

- **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 Michael Schiller
  Co-PI: Denis Vyalikh (DIPC)

- **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

- **Retos Investigación 2017, MAT2017-88377-C2-2-R**
  Transistores de spin basados en heterostructuras Van der Waals
  PI: Sara Barja Martínez
  Co-PI: Miguel Moreno Ugeda (DIPC)

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

- **Contratos Personal Técnico de Apoyo (PTA) 2017, PTA2017-14359-I**
  Técnico para el laboratorio de rayos X del CFM (CSIC-UPV/EHU): mantenimiento del servicio y explotación de nuevas oportunidades de los equipos
  Supervisor: Arantxa Arbe Mendez

- **Contratos Ramón y Cajal (RyC) 2017, RYC-2017-21931**
  Novel physical phenomena in two-dimensional materials
  PI: Sara Barja Martinez

- **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

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

- **Proyectos de I+D+i Retos investigación 2018 (RTI2018), RTI2018 097895 B C44**
  FUN-SOC - Novel Functionalities Driven by Spin-Orbit Interactions
  PI: Nicolás Lorente Palacios
  Co-PI: Deung-Jang Choi

- **Proyectos de I+D+i Retos investigación 2018 (RTI2018), RTI2018 098554 B I00**
  E-CRETE - Energy storage solutions based on ConCRETE
  PI: Jorge Sánchez Dolado
  Co-PI: Juan José Gaitero Redondo (Tecnalia)

- **Proyectos de I+D+i de Generación de Conocimiento 2018 (PGC2018), PGC2018-094548-B-I00**
  SONIBOND - Tailored Soft Nano-Objects Based on Intrachain Bonding: From Design to Materials
  PI: Ángel Moreno Segurado
  Co-PI: José A. Pomposo Alonso

- **Redes Investigación 2018 - Red Temática, RED2018-102752-T**
  NANOLIGHT.es - Light Control on the Nanoscale
  PI: Javier Aizpurua Iriazabal

SPANISH MINISTRY RESEARCH PROJECTS AND NETWORKS

- **Redes Investigación 2018 - Red Temática, RED2018-102833-T**
  OSMolSis - Ciencia Molecular en Superficies: Síntesis y Funcionalidad
  PI: Daniel Sánchez Portal

- **Redes Investigación 2018 - Red Temática, RED2018-102459-T**
  CAT&SCALE - (Photo-) Electrocatalysis: from the Atomic Scale to Advanced Devices
  PI: Sara Barja Martinez (network coordinator)

- **Adquisición de Equipamiento Científico-Técnico 2019, EQC2019-005735-P**
  Installation of a liquid Helium recovery and supply plant for cryogenic experimental systems
  PI: Martina Corso

- ***CSIC* – II Edición del Programa "Cuenta la Ciencia", FGCC-2019-0003**
  Creativium
  PI: Gustavo Schwartz Pomeraniec

- ***CSIC* – I-LINK+ 2018, Red de Internacionalización, LINKB20012**
  NEXTWATER-ilink - Network Exchanges Training program on dynamics and nanostructure of biomolecules in WATER solutions
  PI: Silvina Cerveny Murcia

- ***CSIC* – Fondo de Apoyo a los Servicios Científico Técnicos (FAS) 2019, FAS_19_0297**
  Servicio científico-técnico Centro de Cálculo de Altas Prestaciones - Mejora del sistema de climatización del Centro de Proceso de Datos 2 (CPD-2)
  PI: Iñigo Aldazabal Mensa

- ***CSIC* – Programa de Apoyo a la Infraestructura (PAI) 2019-2020, PAI 06-3356**
  Implementación del nuevo laboratorio de síntesis
  PI: Javier Aizpurua Iriazabal

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

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

- **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

- **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 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

- **Princeton Internationalisation Fund (IF)**
  ## Understanding and Exploiting Nanostructured Soft Materials Network
  PI: Daniele Cangialosi

- **"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), GA 800923**
  ## SUPERTED - Thermoelectric detector based on superconductor-ferromagnet heterostructures
  PI: 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

- **COST Action, CA17139**
  ## EUTOPIA - European Topology Interdisciplinary Action
  PI: Ángel Moreno Segurado

- **Marie Curie Individual Fellowship (H2020-MSCA-IF-2017), GA 797109**
  MagicFACE - Magnetic Hybrid Metal-Organic Interfaces
  Supervisor: Enrique Ortega Conejero

- **ERC Starting Grant (ERC-2018-STG), GA 802533**
  SuperH - Discovery and Characterization of Hydrogen-Based High-Temperature Superconductors
  PI: Ion Errea Lope

- **FET-OPEN – Novel ideas for radically new technologies (H2020 FETOPEN 01-2018 2019 2020), GA 829067**
  THOR - Terahertz detection enabled by molecular optomechanics
  PI: Javier Aizpurua Iriazabal

- **Leadership in Enabling and Industrial Technologies, Space (H2020 SPACE 11 TEC-2018), GA 821932**
  SMART-FLEX - Next generation metamaterial-based SMART and FLEXible optical solar reflectors
  PI: Javier Aizpurua Iriazabal

- **EIG CONCERT – Japan 5th Joint Call, Functional Porous Materials, PCI2019 103657**
  POROPCM - Functional POROus centitious nanocomposites for heat storage in buildings using Phase Change Materials
  PI: Jorge Sánchez Dolado

- **Marie Curie Individual Fellowship (H2020-MSCA-IF-2018), GA 839237**
  PhotoWann - Bulk Photovoltaic effect via Wannier functions
  Supervisor: Ivo Souza

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 Cooperative Research Centers (CICs) launched by the Basque Government.

The portfolio of contracts and collaboration agreements with different companies or external parties has been very productive during 2019. Some examples of the partners involved are:

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

Baskrete cross-border initiative
Concrete science and technology

Michelin (France)
Understanding of "plasticizer effect" on concentration fluctuations and broadening of glass transition in dynamically asymmetric mixtures of interest for tire formulation

Mujeres por África Foundation
ELLAS INVESTIGAN project (V edition) to promote the leadership of African women in scientific research and technology transfer.
LEARN AFRICA scholarship program for African women students

Asociación de Divulgación Científica Pint of Science España
Promotion of Pint of Science 2019 festival in Donostia / San Sebastián

Kutxa Fundazioa
Scientific cultural activities

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 start-up **BihurCrystal**, which is dedicated to the design of ultra-high vacuum (UHV) technologies and new materials for scientific research. BihurCrystal and CFM research groups collaborate regularly and are developing several R+D+i projects together (***e.g.*** H2020 FETOPEN – SUPERTED (GA 800923) or INTERREG POCTEFA – TNSI (EFA194/16/TNSI)).

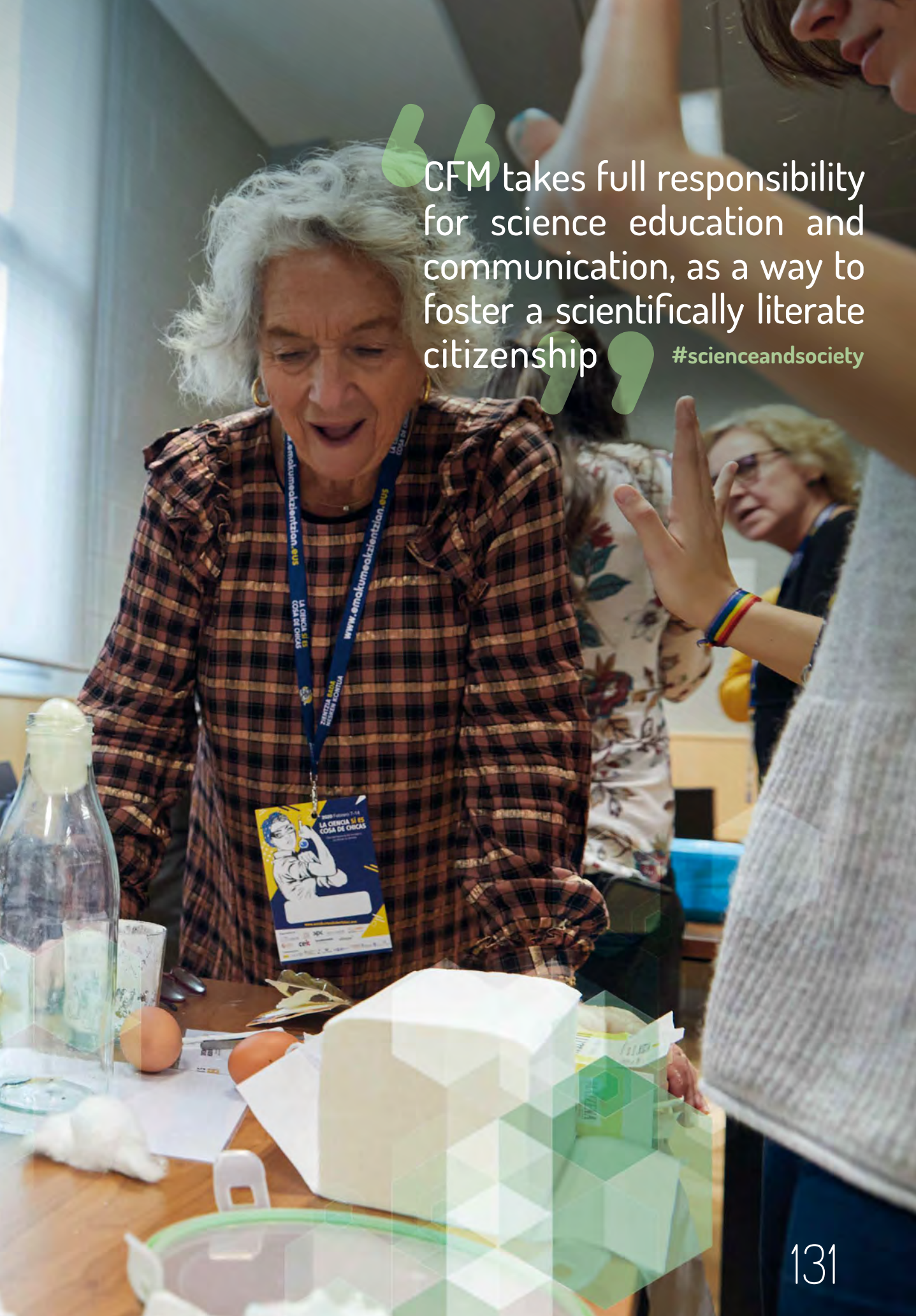
BihurCrystal
www.bihurcrystal.com

SCIENCE AND SOCIETY

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, post-doctoral researchers, to pre-doctoral researchers and science communicators.

The efforts at CFM have been devoted to achieve mainly two objectives: (i) spreading scientific culture and (ii) generating scientific vocation. Since the Gender Equality Plan was designed (see section, Gender Equality at CFM), we have also included the gender perspective in all the activities organized, trying to maximize the visibility of our women researchers, ensuring the gender balance in the talks organized and promoting the awareness on the situation.

Within this spirit, CFM implemented a complete scientific outreach program, and during 2019 more than 40 activities and events were organized, many of them in collaboration with other institutions.



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

#scienceandsociety

SCHOOL VISITS

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 school students, approximately every two weeks during the academic year.

During 2019, CFM had the pleasure to host a total of 16 visits, receiving 549 students, with more than 25 top-line researchers involved in this activity. The calendar of visits during 2019 is displayed below:

JANUARY	FEBRUARY	MARCH	APRIL
La Asunción Ikastetxea (Donostia/San Sebastián)	**Summa Aldapeta** (Donostia/San Sebastián)	**San Benito Ikastola** (Lazkao)	**Lekaroz BHI** (Lekaroz)
Zubiri-Manteo BHI (Donostia/San Sebastián)	**Urretxu-Zumarraga Ikastola** (Urretxu)	**Toki Ona BHI** (Bera)	**Philosophy Faculty** (Donostia/San Sebastián)
		Farmazia Fakultatea (Vitoria-Gasteiz)	**Aita Larramendi Ikastola** (Andoain)

MAY	OCTOBER	NOVEMBER	DECEMBER
Axular (Donostia/San Sebastián)	**IES Hernani** (Hernani)	**Aita Larramendi Ikastola** (Donostia/San Sebastián)	**Lekaroz BHI** (Lekaroz)
	Santa Maria Ikastetxea (Donostia/San Sebastián)	**Aranzadi Ikastola** (Donostia/San Sebastián)	

ZIENTZIA AZOKA

BILBAO
11 May 2019

Elhuyar Zientzia Azoka is a public fair of science projects that takes place yearly in Bilbao. Opened to the public like a big market, it gathers 90 projects developed by more than 300 young students, coming from 31 schools. It is a unique opportunity to learn from within scientific research and technological development, and to promote the scientific culture among the society. CFM is one of the multiple agents of the scientific and technological network of the Basque Country that collaborate in its development.

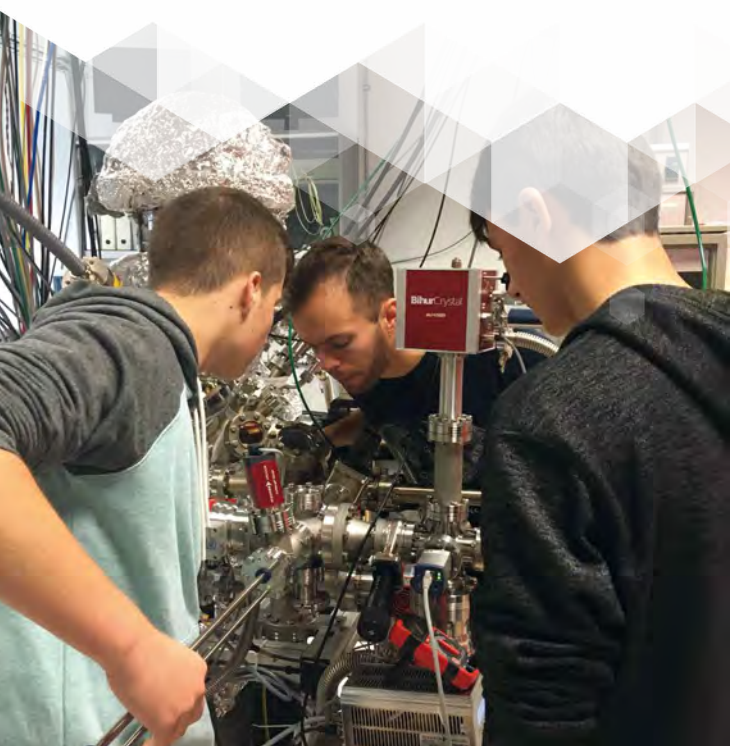
In this 2019 edition, CFM helped mentoring the projects, and during the actual fair joined the selection committees that gave the awards and supported the communication campaign.

In addition, CFM offered two of the prizes for the young winners, consisting in a stay of two days at CFM, hosted by top of the line researchers.

CFM prize winner schools: La Salle Bilbao and Begoñazpi Ikastola

Jury members from CFM at Zientzia Azoka: Nerea Zabala, Amaia Iturrospe and Idoia Mugica

Hosts of the winner teams at CFM: Lucia Vitali, Celia Rogero, Gabriel Molina, Daniel E. Martínez Tong, Daniel Arismendi and Ester Verde



XVI SCIENCE WEEK (UPV/EHU)

TABAKALERA, DONOSTIA / SAN SEBASTIÁN
7-9 November 2019

Inside the Materials World Stand

From the 7th to the 9th of November 2019, CFM together with DIPC and CIC nanoGUNE, joined the UPV/EHU's science week with the stand "Inside the Materials World" at ***Tabakalera*** cultural center in Donostia / San Sebastián.

Master students, as well as pre-doctoral, 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.

"A LIFE IN SCIENCE" IN EUREKA! ZIENTZIA MUSEOA

EUREKA! ZIENTZIA MUSEOA, DONOSTIA / SAN SEBASTIÁN
21 October and 4 November 2019

Since 2010, ***Eureka! Zientzia Museoa*** (the science museum in Donostia / San Sebastián) organizes a meeting that 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 by participating actively with researchers of different backgrounds of the center who share their experiences.

In 2019, the following researchers from CFM joined this activity, attended by more than 300 students and 50 professionals:

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

  Poster: Fisikari teoriko-konputazional baten "laborategia"

- **Gabriel Molina**
  Talk and Poster: Mi vida científica

- **Daniel J. Arismendi**
  Talk and poster: Yo trabajo en un laboratorio virtual y mis experimentos se hacen en un superordenador

- **Daniel E. Martínez-Tong**
  Poster: Así se ve un plástico a través de un microscopio avanzado...

- **Martina Corso**
  Poster: ¿Cómo se puede ver el mundo en la nanoescala?

- **Laura Fernández**
  Poster: Superficies nanoestructuradas

JAKIN-MINA: THE WORLD OF TINY THINGS

JAKIUNDE - CIC NANOGUNE
22 March, 2019

Conference by Sara Barja in the framework of the program Jakin-mina organized by the arts and science academy Jakiunde devoted to high school students.

OPENING OF THE XXXVIII EDITION OF THE UPV/EHU SUMMER COURSES

MIRAMAR PALACE, DONOSTIA / SAN SEBASTIÁN
19 June 2019

On the official opening of the UPV/EHU summer courses, Javier Aizpurua, head of the "Theory of Nanophotonics" group at CFM and DIPC, was invited to give a master class called "When light becomes small".

DONOSTIA WEEKINN 2019

BAGA BIGA FAKTORIA, DONOSTIA / SAN SEBASTIÁN
29 October 2019

CFM researcher Aitor Bergara participated in the 6th Innovation Week (Donostia weekINN 2019) organized by ***Fomento*** of Donostia / San Sebastián with the following outreach talk:

Zientzia & Fun Fútbol & Ciencia / Futbola & Zientzia

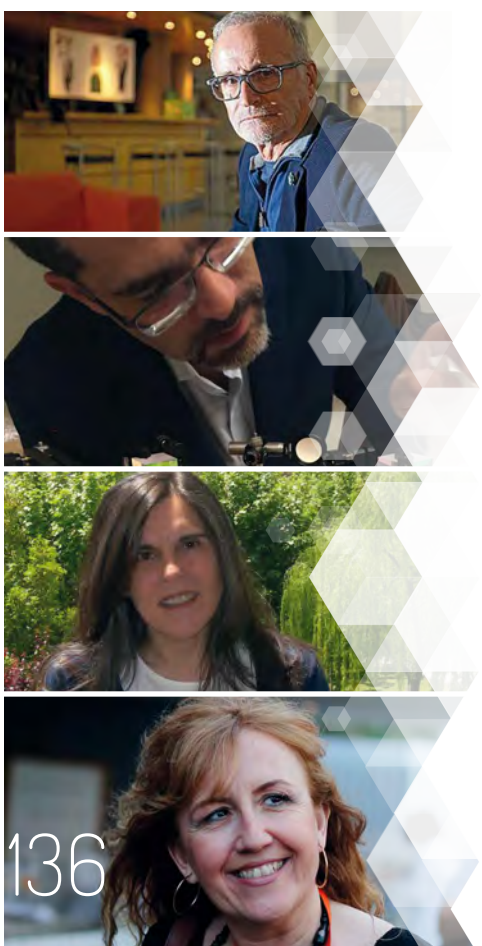
"QUÉ SABEMOS DE..." TALK SERIES

KUTXAKULTUR PLAZA AT TABAKALERA, DONOSTIA / SAN SEBASTIÁN
8, 15, 22 and 29 November 2019

Qué sabemos de... is a peculiar series of outreach talks inspired by the intrinsic curiosity of the human being. The program, yearly organized by CFM and CSIC since 2017, takes place at the iconic cultural center ***Tabakalera*** in Donostia / San Sebastián, with the collaboration of ***Kutxakultur.***

Available at CFM's YouTube channel or scanning this code

More than 400 attendees participated in the 4 talks that included hot topics and renowned speakers.



Inteligencia Artificial
Ramón López de Mántaras

CSIC Researcher at *Instituto de Investigación en Inteligencia Artificial* (IIIA), Barcelona

El mundo cuántico
Gabriel Molina Terriza

Ikerbasque Professor and leader of the Quantum Nanophotonics Laboratory at CFM

El Chocolate (Biología y nutrición)
Mª Ángeles Martín Arribas

CSIC Tenured Scientist at *Instituto de Ciencia y Tecnología de Alimentos y Nutrición* (ICTAN), Madrid

Clima y humanos. Una larga historia de amor/desamor desde la prehistoria
Penélope González Sampériz

CSIC Researcher at *Instituto Pirenaico de Ecología* (IPE-CSIC), Zaragoza

PINT OF SCIENCE

DONOSTIA / SAN SEBASTIÁN
20-22 May 2019
pintofscience.com

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, since 2018, CFM supports this festival that fills up our city with science. Cheers!!!

In the framework of this festival, in 2019, two CFM researchers participated with the following talks:

Supereroankortasuna marka guztiak hausten!
Ion Errea Lope

Plástico: una historia de amor y desengaño
Paula Malo de Molina Hernández

PRIDE IN STEAM DAY

CONVENT GARDEN, DONOSTIA / SAN SEBASTIÁN
5 July 2019

CFM, together with DIPC and CIC nanoGUNE, organized the first day of Pride in Science day in Donostia / San Sebastián with two scientific dissemination talks addressing the LGTBQI transversal topic.

With this initiative, CFM joined the international movement PrideinSTEM (Science, Technology, Engineering, and Mathematics) that, for some years now, seeks to give visibility to the LGTBIQ collective in science. The message is loud and clear: in science too, diversity is essential.

Ciencia LGTBIQ ¿Algún problema?
Aitzol García-Etxarri

Azul, rosa u otra cosa
Isabel López-Calderón

Available at CFM's YouTube channel or scanning this code

16TH EDITION OF PHOTO EXHIBITION "FOTCIENCIA"

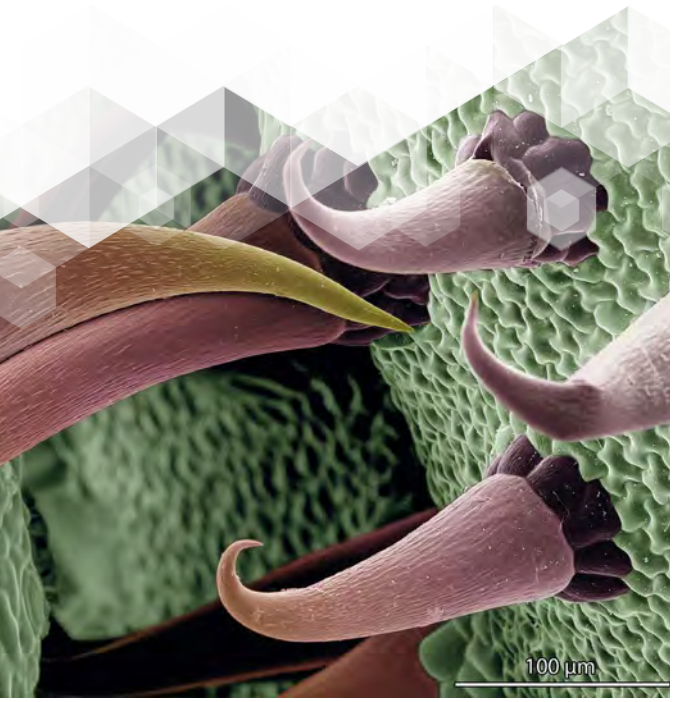
CRISTINA ENEA FOUNDATION, DONOSTIA / SAN SEBASTIÁN

2-30 September 2019

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 2019, and CFM had the pleasure to host it in Donostia / San Sebastián, continuing with the tradition implemented for the last four years.

In 2019 the exhibition was opened to the public from the 2nd 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, DONOSTIA / SAN SEBASTIÁN

14 September 2019

How far do our eyes see? With this moto, around 25 kids and their families participated in this workshop guided by CFM researchers and experts in the field. The explorers discovered the world of macro, micro and nanoscopic scales, by collecting samples in the park of ***Cristina Enea*** and putting them under a homemade microscope and different magnifying glasses.

INTERNATIONAL WOMEN AND GIRL IN SCIENCE DAY 2019

CIC NANOGUNE, CIC BIOMAGUNE, DIPC AND CFM
11-15 February 2019

SCIENCE IS INDEED A GIRLS' 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' in Science Day.

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 onboard, the 4 centers joined forces to present a full week program that aimed women teenagers, school kids, elder women (above 55), citizens in general and the scientific community.

DO YOU KNOW ANY WOMEN IN SCIENCE?

February 11, CIC BiomaGUNE, Primary School kids (10-11 years old)
February 11, DIPC and CFM, High School students (16-18 years old)
February 12, CIC nanoGUNE, Primary School kids (10-11 years old)

50 Students in of primary school participated in the workshops at CIC biomaGUNE and CIC nanoGUNE, carrying out different activities and scientific demonstrations aimed at highlighting the role of women in science throughout history.

Meanwhile, DIPC and CFM hosted the visit of 45 high school students through a tour into the laboratories and computing center. Exclusively women researchers of these centers guided the visit, allowing the students to interact directly with them.

HAND IN HAND

Koldo Mitxelena, Donostia / San Sebastián
February 11
Open talk

Over 60 people attended this event where some of the most avant-garde and brilliant research projects developed at CIC nanoGUNE, CIC BiomaGUNE, DIPC and CFM research centers where presented. The leadership in all of them resides in both a woman and a man working as a team.

- **Reyes Calvo** (CIC nanoGUNE) & **Miguel Moreno** (DIPC-CFM)
- **Celia Rogero** (CFM) & **Sebastián Bergeret** (DIPC-CFM)
- **Aitziber López Cortajarena** (CIC biomaGUNE) & **Fernando López** (CIC biomaGUNE)

Available at CFM's YouTube channel or scanning this code

OPEN SCIENCE FROM THE INSIDE OUT: CONCEPT, CHALLENGES AND IMPLEMENTATION BY EVA MÉNDEZ

Carlos Santamaria Center UPV/EHU, Donostia / San Sebastián
February 13
Open talk addressed to the Scientific Community

Eva Méndez, Deputy Vice President for Scientific Policy-Open Science at UC3M and member of the EU-OSPP (European Open Science Policy Platform) on behalf of YERUN (Young European Research Universities Network), approached the concept of 'Open Science' from the reflection of ideas and policies discussed in the context of the European Union, but also addressing the challenge of implementation for the different agents involved. The main initiatives launched in this area (PlanS, OSPP-REC, etc.) as well as the barriers to the necessary cultural change were discussed.

Available at CFM's YouTube channel or scanning this code

AMONA'S POWER

CFM and DIPC

February 14

Workshop and visit addressed to +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 the workshop, sharing a unique experience with all the volunteers.

The success of this workshop led the science association from Ondarroa, ***Zientziaren Giltzak***, to invite CFM to organize ***Aume's Power*** in their village, in the context of the science week they celebrate in May. More than 30 women from this town participated in this fun and enriching meeting.

SCIENCE IS INDEED A GIRLS' THING

CIC nanoGUNE

February 15

Workshop addressed to teenage women

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

CREATIVIUM

creativium.mestizajes.es

Gustavo A. Schwartz, a CSIC researcher at CFM, associated to the DIPC, launched the project Creativium, in the framework of the Mestizajes program, promoted by DIPC and directed by Gustavo as well.

Creativium is a project based on three pillars: a photobook, a photographic exhibition and a website. The photographs were taken by Paula Arbide to scientists from DIPC, CFM and CIC nanoGUNE. The photographic exhibition was inaugurated on 23rd September 2019 in Donostia / San Sebastián. It has been conceived as a traveling exhibition that can be presented throughout Spain (and eventually also internationally). The book has been published in three languages (Spanish, English and Basque), although only the Spanish version has been commercialized so far through ***Los Libros de la Catarata.*** In November 2019, the presentation of the book ***Creativium*** took place at the FNAC bookstore in Donostia / San Sebastián. The website centralizes the entire project and serves to promote the book and future exhibitions.

The three formats to present the project were chosen with the aim of seducing the public from the aesthetic value of the images and creating a sense of familiarity that allows us to naturally understand both the role of creativity in the scientific activity and the mechanisms of the creative process and the scientific study of creativity.

INSPIRACIENCIA

Inspiraciencia is a contest of scientifically inspired stories organized yearly by the CSIC delegation in Catalonia, and supported by the ***Fundación Española para la Ciencia y la Tecnología*** (FECYT).

In 2019 CFM collaborated with this initiative, constituting the jury of the Basque written stories category and helping in the organization of the award giving ceremony that took place in the Aquarium of Donostia / San Sebastián. In this ceremony Gustavo A. Schwartz, CSIC researcher at CFM and creator of the program ***"Mestizajes: Enredando Ciencias y Humanidades"*** at DIPC, offered a talk on the journey from the Big Bang to consciousness through science and literature.

PASSION FOR KNOWLEDGE P4K

p4k.dipc.org/en/home

The **Passion for Knowledge** (P4K) festival is a collective celebration of learning and curiosity, involving the active participation of **thousands of citizens**. This festival is organized by DIPC and is held mainly in Donostia / San Sebastián. CFM collaborated in the organization, being specially involved in two events: ***Encounters with Nobel Laureates*** and ***Passion Txiki.***

ENCOUNTERS WITH NOBEL LAUREATES

2 October 2019, Donostia / San Sebastián

4 October 2019, Bilbao

In this encounters, Nobel Laureates and world-leading researchers meet secondary school students. The main aim of these encounters is to foster students' interest in science and technology, and to kindle a passion for knowledge in their young minds.

In Donostia / San Sebastián, the invited researchers were the astrophysicist Dame Jocelyn Bell Burnell, the chemist Jean Pierre Sauvage (Nobel Prize in Chemistry 2016) and the theoretical physicist Ignacio Cirac, and in Bilbao, the physicist Albert Fert (Nobel Prize in Physics 2007), the paleoanthropologist María Martinón and the experimental physicist Cristopher Rossel.

PASSION TXIKI

Club Room at Victoria Eugenia, Donostia / San Sebastián

5 October 2019

CIC nanoGUNE and CFM coordinated the organization of ***Passion Txiki,*** the mini science festival targeted at children and their families. 120 kids participated in the set of activities that included a range of fun live experiments, scientific storytelling and games.

CINEMA AND SCIENCE

DONOSTIA / SAN SEBASTIAN AND BILBAO

The second edition of the cinema and science cycle was organized by the Basque Film Archive and DIPC at the Bilbao Fine Arts Museum (Bilbao) and in Tabakalera (Donostia / San Sebastián). Under the name "The Unknown", the program included 12 film projections presented by prestigious scientists, a special event in collaboration with Bang Bang Cinema, together with sessions for scholars and public talks. It is estimated that more than 4,600 people participated in the projections and events

Javier Aizpurua and Ion Errea, researchers at CFM, participated presenting the following films:

Blade Runner (Ridley Scott, 1982) + Blade Runner 2049 (Denis Villeneuve, 2017)

2 and 16 March 2019

Presented by Javier Aizpurua

Hidden Figures (Theodore Melfi, 2016)

13 and 20 March 2019

Presented by Ion Errea as part of the scholar sessions physicist

ACTIVITY IN MASS MEDIA

During 2019, CFM was cited over 148 times in the media, including press, online articles, TV and Radio.

Press articles
55*

Online press
58*

Radio
32

TV
1

*Scientific publications excluded

An example of this intense activity is Ion Errea's collaboration with ***Udako Faktoria*** program that continued throughout the summer on a weekly basis. Moreover, since October CFM has a permanent section "Breakfast with Science" in the ***Goiz Kronika*** program of ***Euskadi Irratia,*** run every Sunday by Idoia Mugica, head of communication and dissemination of CFM, while the collaboration with the well-known science outreach radio program ***"La Mecánica del Caracol",*** in ***Radio Euskadi*** (EITB), is still ongoing. 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.

@CFMDONOSTIA

CFM is also present and active online and in the social media, and can be officially found in Twitter, Facebook, Instagram, Youtube and, since January 2020 in LinkedIn, as well as in our own CFM website.

As of February 2020, we had 720 followers in Twitter, 250 in Facebook and 115 in Instagram, while the community of LinkedIn is also growing. CFM's Youtube channel already contains more than 20 videos featuring different events. Besides, the CFM website is very regularly updated with news, workshops, seminars, and much more, especially our Job Offers section, which is of great interest for many of our visitors and receives very high traffic.

Receive updated information about the activities and events we organize at CFM devoted to the general and scholar public **subscribing here** and stay tuned following us in our social media channels.

OUTREACH COLLABORATION NETWORK

CFM has established strategic alliances regarding scientific outreach initiatives which create important synergies. These are the CFM's main partners 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 Foral de Guipúzcoa / Gipuzkoako Foru Aldundia

Aulas Kutxa - kutxakultur

Eureka! Zientzia museoa

Norteko Ferrokarrila eta Zientzia Azoka (Elhuyar Fundazioa)

La Mecánica del Caracol (Radio Euskadi)

Goiz Kronika eta Udako Faktoria (Euskadi Irratia)

Pint of Science

FECYT

Cátedra de Cultura Científica (UPV/EHU)

Berritzegune Nagusia

Pride in STEM

MISCELLA-NEOUS

PHD RECRUITMENT FAIR 2019

In 2019 CFM organized the second 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, 7 candidates were selected and granted full studentships to join one research group at CFM:

- **Agustín Blázquez Martín**
  Group: Polymers and Soft Matter
- **Alfredo Serrano Jiménez**
  Group: Gas/Solid Interfaces
- **Bruno Candelas Peñalba**
  Group: Theory of Nanophotonics
- **Elia Turco**
  Group: Nanophysics Lab
- **Javier Martínez Sabando**
  Group: Polymers and Soft Matter
- **Martin Gutiérrez Amigo**
  Group: Quantum Theory of Materials
- **Matteo Sanviti**
  Group: Polymers and Soft Matter

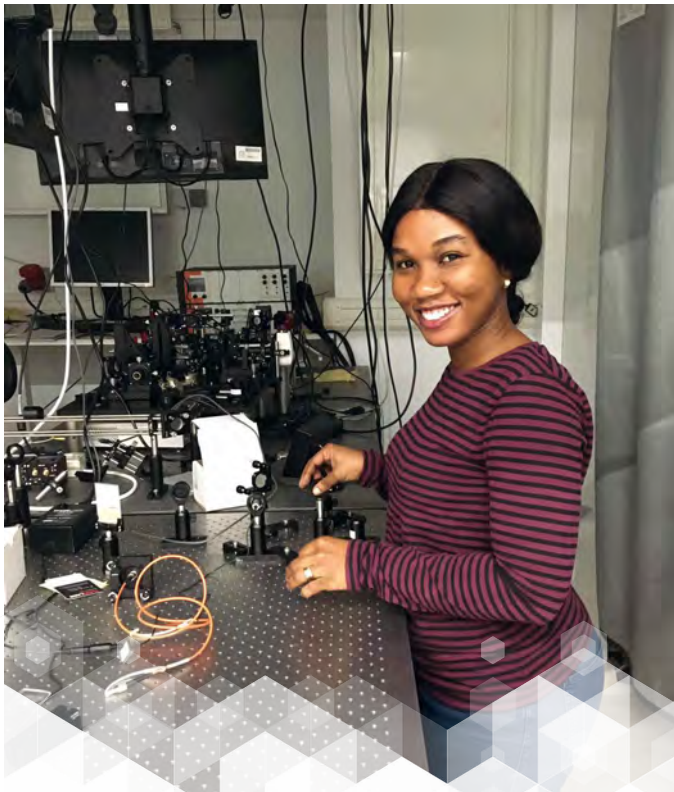
CFM AND WOMEN FOR AFRICA

GIPUZKOA COOPERA PROGRAM WITH THE WOMEN FOR AFRICA FOUNDATION, DIPC, 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. CFM has been part of the program since its very beginning, and the last two years it has materialized in a collaboration with the foundation Women for Africa.

The aim of the initiative is facilitating the professional growth of African women scientists and entrepreneurs through temporary residencies in research centers of reference in Gipuzkoa, so that they can broaden their knowledge and then apply it in their country of origin.

Thanks to this initiative, in the framework of the program "Science by Women" promoted by the foundation Women for Africa, two African researchers carried out six-month research stays at DIPC and CFM during 2019. The Provincial Council of Gipuzkoa financed each of these long stays with 25 000€. The female African researcher visiting and collaborating at CFM was Dr. **Jetro Epse Njukeng Nkengafac** from Cameroon who joined the Polymers and Soft Matter group, hosted by Prof. Ángel Alegría. In 2020, **Aline Simo** from Cameroon will join Jorge Sánchez Dolado's team at the Ceramic and Cement- Based group of CFM.



LEARN AFRICA

Together with the "Science by Women" 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 young African women students through scholarships in Spanish universities that collaborate in this initiative.

Since 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 program of the UPV/EHU. In 2019, the recipient of the scholarship was Harriet Kumi from Ghana, who is currently developing her Master Thesis at CFM under the supervision of Gabriel Molina at the Quantum Nanophotonics Lab.

EUSKADI RESEARCH PRIZE

PROF. EUGENE TCHOULKOV

In 2019, Professor Eugene Tchoulkov, professor in the Department of Materials Physics at the UPV/EHU (2003), and researcher at CFM and DIPC, received the Euskadi Research Prize 2018, the maximum recognition given in the Basque Country in the field of sciences. The Court of the twenty-third edition of the Prize, made up of five members of recognized prestige in the field of Science and Technology, unanimously agreed to award the prize to the physicist of Russian origin living in the Basque Country, after deliberating among the ten candidates presented in this edition.

The winner, according to the jury, "has made an extraordinary contribution to the study of solid state and surface physics and to the creation of a renowned school of scientific excellence in the Basque Country".

The Department of Education annually announces the Euskadi Research Prize. In even years, as is the case (2018), the prize corresponds to the area of Science and Technology, while in odd years it is dedicated to the recognition of the work of professionals in the area of Social Sciences and Humanities. The aim of the Euskadi Research Prize is to encourage scientific activity and to stimulate, promote and value the efforts of qualified researchers and teams whose work has had a significant positive influence on the Autonomous Community of the Basque Country.

HIPATIA – MUJERES EN LA CIENCIA AWARD 2019

DR. SARA BARJA

In 2019 elEconomista held the first edition of the Hipatia - Mujeres en la Ciencia awards, an initiative that aims to recognize women who have contributed the most to the advancement of research or scientific progress in Spain during the year. This prize acknowledges young talent in science among women scientists whose aptitudes and merits to date prefigure a greater projection in research within their field of specialization.

The winners in this first edition have been two doctors, Sara Barja and Elena García, and Clara Piloto, a high executive. Sara Barja, is currently a researcher at the Nanophysics Lab at CFM and after being appointed Ikerbasque Fellow, she currently holds a Ramon y Cajal contract with the UPV/EHU.

The organization highlighted that all of the winners have a great track record and a bright future that stands out thanks to their commitment to the development of science, social welfare and equality between men and women.

HIGHLY CITED RESEARCHER 2019

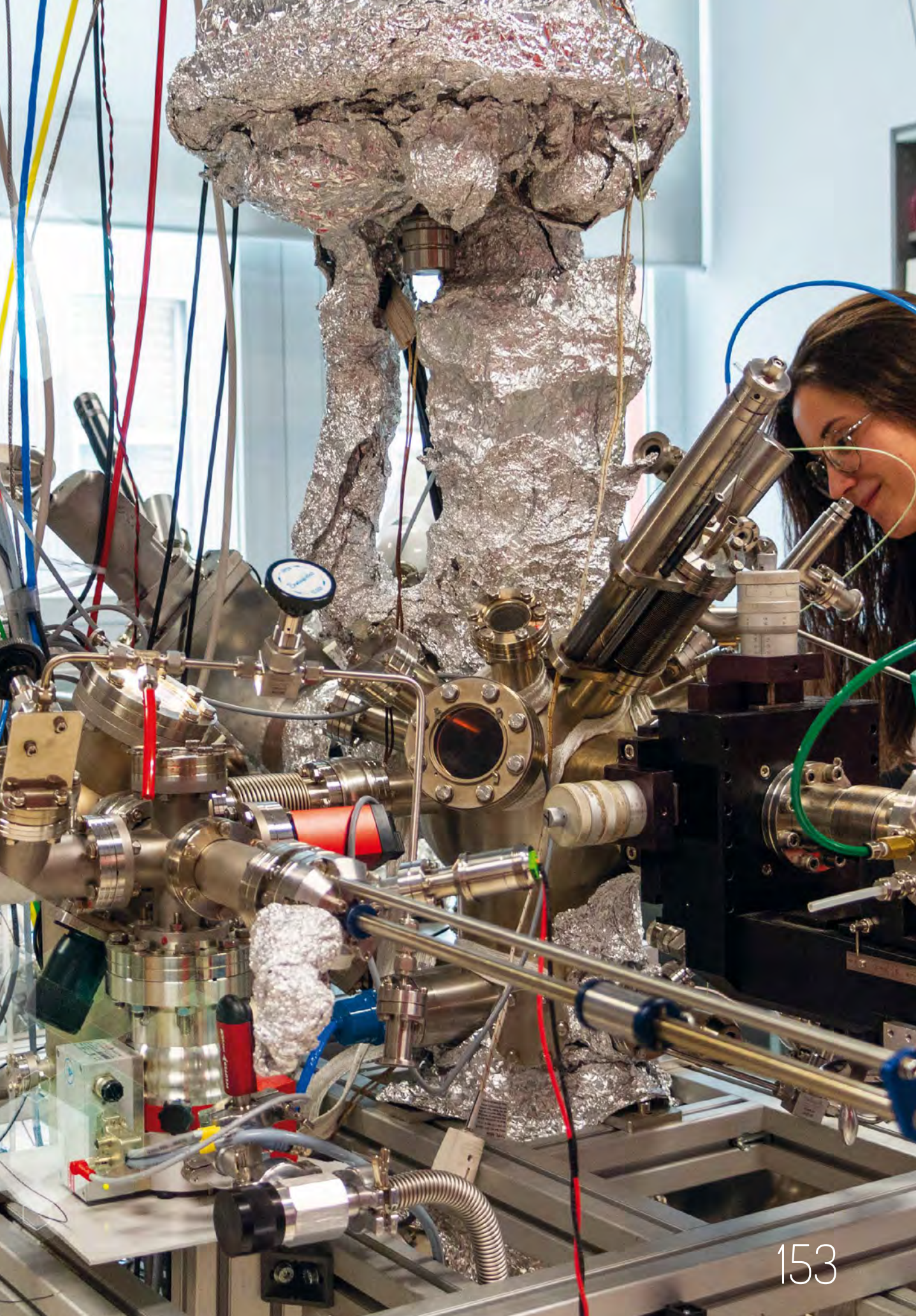
PROF. JAVIER AIZPURUA IRIAZABAL

After being included for the first time in 2017, Professor Javier Aizpurua remains in the 2019 list of the most cited researchers in the world for the third year in a row, according to the database drawn up by Clarivate Analytics. Prof. Javier Aizpurua is head of the "Theory of Nanophotonics" group at CFM and DIPC. 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.

GENDER EQUALITY AT CFM

The European Commission (EC) in its last 'She Figures' report warned that the low representation of women in the science sector, both in public and private institutions, and especially in senior positions, remains a major problem in all EC member states. The Basque Country is no exception, and presents this same situation, as reflected in the reports on the subject that Ikerbasque has been carrying out.

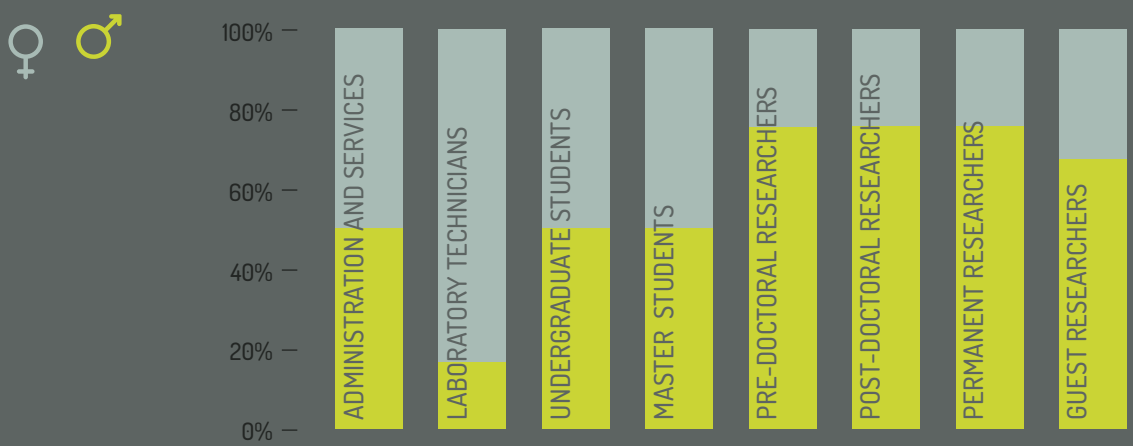
In 2019 CFM fulfilled an exhaustive process of analysis of the internal situation, which included a compilation of its own indicators on gender balance, in order to make an internal diagnosis of the center's gender situation.



GENDER EQUALITY

	MEN	WOMEN	
ADMINISTRATION AND SERVICES	7	7	**14**
LABORATORY TECHNICIANS	1	5	**6**
UNDERGRADUATE STUDENTS	5	5	**10**
MASTER STUDENTS	3	3	**6**
PRE-DOCTORAL RESEARCHERS	46	15	**61**
POST-DOCTORAL RESEARCHERS	34	11	**45**
PERMANENT RESEARCHERS	31	10	**41**
GUEST RESEARCHERS	37	18	**55**
	164	74	**238**

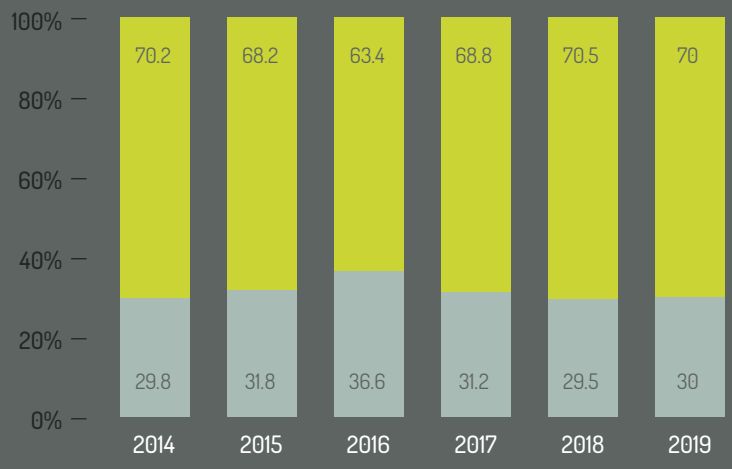
Staff distribution at CFM according to category and gender (percentage)



Regarding the evolution of the gender distribution of CFM scientific staff (including technical staff) it has remained at a ratio of about 30/70 (women/men) over the past years. These data are consistent with the data provided by the CSIC in its annual report on women and science.

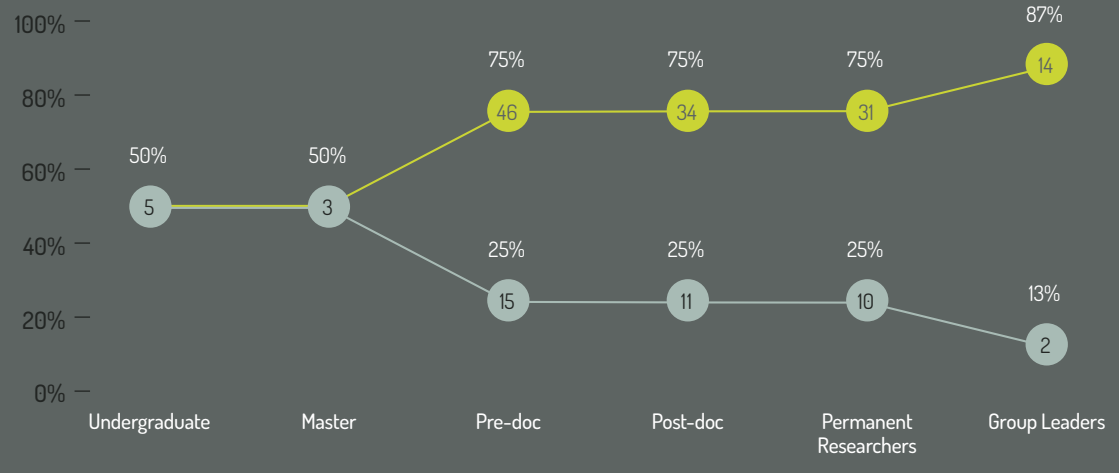
> CFM scientific staff (including technical staff) has remained at a ratio of about 30/70 (women/men) over the past years

Evolution over the years of the gender distribution (percentage) of the scientific and technical staff of the CFM



The next figure shows the percentage of women and men in different research positions. This analysis states that the disproportion in the distribution of women/men in the center starts already at the earliest stage of the scientific career. Currently, less than 25% of the pre-doctoral researchers at CFM are women. The gender imbalance is accentuated as the responsibility for the job and level in the research career is greater, corroborating the general trend observed in the Basque Country and Europe.

Distribution of scientific staff of CFM, according to category and gender (until December 31, 2019)



FIRST GENDER EQUALITY PLAN OF CFM

CFM has assumed the responsibility for alleviating gender inequality, and has shown its commitment by designing the first CFM Gender Equality Plan (GEP).

In 2017, the design and implementation of this specific Gender Equality Plan was proposed for the center, which finally materialized in 2019, with the support of the services offered by "Elhuyar Aholkularitza". Elhuyar coordinated the European project PLOTINA (GA 666008) of the call H2020-GERI-2014-1 to support to research organizations to implement gender equality plans. The Regional Government of Bizkaia has accredited Elhuyar since 2005 to provide technical assistance in the field of equal opportunities and gender policy. Elhuyar has also been collaborating with Emakunde since 2008.

The development and implementation of the GEP included four (4) stages:

1. Analysis stage (2018-2019 completed), for the collection of center data disaggregated by sex, with the aim of making a critical evaluation of the procedures and practices for the recruitment of staff, support for maternity and paternity leave, etc., and detecting possible gender inequalities and prejudices in the criteria, if any.

2. Planning stage (2019 completed), for the definition of the improvement objectives, and the actions and measures to achieve within the established deadlines, as well as the CFM staff responsible for implementing and monitoring them. An equality commission was set up to carry out this stage.

3. Implementation stage (2020-2023), in which improvement activities will be implemented and dissemination activities will be carried out, in order to expand gradually the commitment of all to gender equality.

4. Monitoring phase, in which the implementation process will be regularly evaluated The results of the monitoring exercises will allow for reorientation, if necessary, of the improvement actions set out in Stage 2, so that the results of the GEP can be optimized.

In mid-2018, the initial phase of the design of the CFM GEP began, which corresponds to the pre-diagnosis of the center's gender situation. In 2019, a gender equality committee was established at the center, made up of researchers, relevant administrative personnel, and the management team. This committee, accompanied and advised at all times by the techniques of Elhuyar aholkularitza, worked on the evaluation of data from the CFM, obtained from the surveys carried out and the extensive work of compiling indicators and documentation carried out in CFM.

Throughout 2019, the GEP was shaped as a specific and exclusive plan of CFM, which reflects the general situation, and brings together all the commitments, actions and will of CFM to cover gender equality in our institution in all its breadth.

At the beginning of 2020, after assuming the changes in the management team, the gender commission was re-established and will be responsible of launching and implementing this plan in the period 2020-2023.

ACTIONS IMPLEMENTED IN 2019

While the CFM GEP will be officially launched in 2020, a series of specific actions to be addressed in the short term were already identified. The aim of those was, among other things, to inform and carry out activities to raise **awareness** of gender issues among the entire center's staff, as well as to the general public, and to **encourage scientific vocations of young women**. The organization of the International Day of Women and Girls in Science, which has been described in depth in section Science and Society of this report, stands out. In addition to this program, specific actions like "Science by women" or "Learn Africa" carried out together with Women for Africa foundation and Gipuzkoa coopera, show the commitment acquired so far (see Miscellaneous section of this report). Nevertheless, it is worth noting that during 2019 CFM did also achieve:

- Ensuring the representation of 50% of women in all the dissemination lectures organized by CFM.
- Encouraging women researchers to participate in the different dissemination programs, especially those aimed at children, families and young people. The list of activities in this line includes visits by schoolchildren to the center, the "Zientzia Azoka-Elhuyar" project and the "A life in science" congress at the Eureka! Science museum, among others.
- Using the CFM social media to highlight the research results of the women scientists working at CFM.
- Promoting other initiatives that share the fundamental contributions of women in science, such as "Women with Science" by Marta Macho (Chair in Scientific Culture), "Women and Girls in Science Day", etc.

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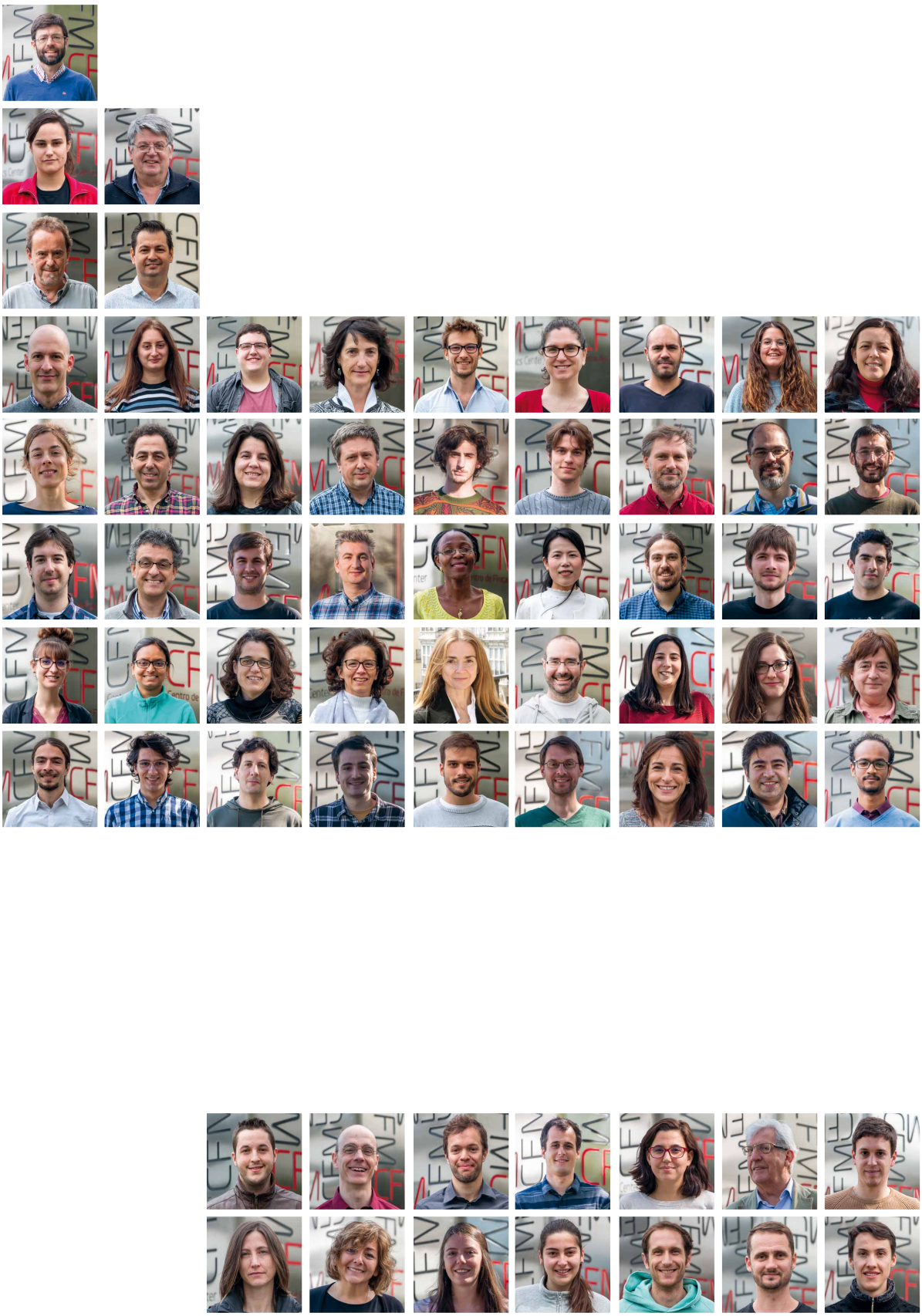
THE ELEMENTS OF CFM



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