Materialen Fisika Zentroa
Centro de Física de Materiales
Materials Physics Center

ACTIVITY REPORT

2020

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 2020

CFM

Centro de Física de Materiales

Materialen Fisika Zentroa

Materials Physics Center

CSIC
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Universidad del País Vasco
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SUMMARY

FOREWORD

Despite all the difficulties, 2020 has been a record year in terms of research output, with an unprecedented number of publications and exceptional quality

Iñaki Juaristi Oliden, Vicedirector

2020 has been a complicated and strange year. For several months, many of us looked around us with a feeling of disbelief, helplessness and sadness as we saw our certainties, routines and, ultimately our way of life tragically transformed due to the Covid-19 pandemic. We have witnessed how many of our neighbors, friends and family were affected and sadly some were unable to overcome it. We have felt fear and loneliness. We have been away from our loved ones, whom we have not been able to comfort and help as we would have liked. All this has left a trace of sadness that is only now beginning to dissipate thanks to the renewed hope brought by advances in the vaccination process and the slow return to normality.

However, from the point of view of science and research activity, the year 2020 has been somewhat more ambiguous. Of course, the pandemic had a negative initial impact. The *Centro de Física de Materiales* (CFM), following the regulation imposed by the University of the Basque Country (UPV/EHU), remained closed and without face-to-face activity for almost two months. During the second half of May, we resumed our activity using a system that combined teleworking with face-to-face activity in shifts, which allowed us to maintain a low occupancy of our facilities. Other measures were imposed, such as the mandatory use of the mask, the closure of communal areas such as the cafeteria and the auditorium, and courses, workshops and scheduled meetings were suspended, etc. Thanks to these measures, and to the discipline and stoicism with which all the staff adopted these measures, it was possible to prevent the appearance of large outbreaks of Covid-19 in the CFM. There have only been isolated cases that were quickly reported, the people involved swiftly confined in their homes, and the possible transmission in the center was avoided. Fortunately, none of these cases had serious consequences. For this civic, responsible and understanding attitude, I want to warmly congratulate all the CFM staff. Finally, in October 2020 the work shifts were definitively abandoned, since they considerably hindered the activity in the laboratories. However, to this day, part of the staff still carries out part of their activities by teleworking.

Despite all these difficulties, 2020 has been a record year in terms of the number of publications (217 articles) and with exceptional quality, as can be seen in this report. It is possible that the pandemic was partially responsible of this, giving us more time to reflect on the results we already had and to finish those manuscripts that were resisting completion. Additionally, there were 82 ongoing research projects (18 of them European and international ones, including one ERC Starting Grant and ERC Advanced Grant), with more than 3,8 million euros granted to CFM researchers only in 2020 and 12 PhD theses defended.

During 2020 our CFM family grew with new members. In April 2020, during the general confinement, Amaia González Azpeitia joined CFM as our new Administration Manager. Despite this unusual start, and the cancellation of several of the training courses organized by CSIC for new administrative personnel, she rapidly got familiar with the center and is progressively taking the

We want to warmly congratulate all the CFM staff for the civic, responsible and understanding attitude shown during this difficult year

Daniel Sánchez Portal, Director

reins of CFM's administration. We wish her the best in this certainly challenging task.

In summer 2020, with an unusually long delay after obtaining their permanent positions, three new CSIC permanent researchers finally joined CFM scientific faculty: Marek Grzelczak, who brings his expertise in the synthesis and characterization of nanomaterials for health care and energy applications to the "Nanomaterials and Spectroscopy" group; Pedro Braña Coto, that applies quantum chemistry methodologies to the field of optoelectronics and molecular physics, and has created the "Theoretical and Computational Chemistry" group in CFM; and Rubén Esteban, an expert in the theory of nanoplasmonics, who has joined the successful "Theory of Nanophotonics" group. Also in summer 2020, we could celebrate that one of our postdoctoral researchers, Julen Ibañez Azpiroz, was awarded an ERC Starting Grant in the 2020 call (that will start in June 2021) with CFM-MPC as its host institution. Julen will create his own group devoted to apply diverse ab initio and theoretical tools to understand in depth the optical and electronic properties of solids. Another reason to celebrate was that our colleague Javier Aizpurua Iriazabal was included for the fourth year in a row in the list of Highly Cited Researchers elaborated by Clarivate Analytics.

Autumn 2020 started with the replacement of Andrés Arnau Pino as Deputy Director of CFM by Iñaki Juaristi Oliden. We really want to thank Andrés for all his great work during the last five years and particularly for his support during the last year, when he had to act both as CFM Deputy Director and Acting Administration Manager. Another important event in Autumn 2020 was the official retirement of our colleague and friend Pedro Echenique Landiribar, a teacher both in science and in life for many of us. He is one the main personalities behind CFM and had a key role in the creation and development of CFM and its research environment (DIPC, nanoGUNE, etc.). He continues with his research, science popularization and science policy advising activities as an Emeritus Professor at UPV/EHU.

As mentioned at the beginning of this foreword, 2020 was a year full of sad moments. For many of us at CFM, a devastating event was the sudden death of our friend and colleague Juan Jose Saenz, Ikerbasque Professor at DIPC, an expert in photonics and optical forces. We miss his kindness and friendly demeanor to all the members of our DIPC-CFM-nanoGUNE community, his generosity, his love of science, and all his good qualities.

The brilliant trajectory and international visibility gained by CFM in the last years was 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. With these allies we are fully confident that we will keep producing basic science at the highest level.

Thank you all for your commitment and support.

Daniel Sánchez Portal
Iñaki Juaristi Oliden

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: **Iñaki Juaristi Oliden**

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.

MPC-BERC

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

PROFILE

SCIENTIFIC COMMUNITY

Researchers in Action

194

18

Research Groups

TRAINING

12

PhD Theses defended

17

Master Theses Defended[1]

3

Undergraduate Projects

RESEARCH OUTPUT

ISI Publications

217

International Collaborations

81%

H Index

133

Citations[2]

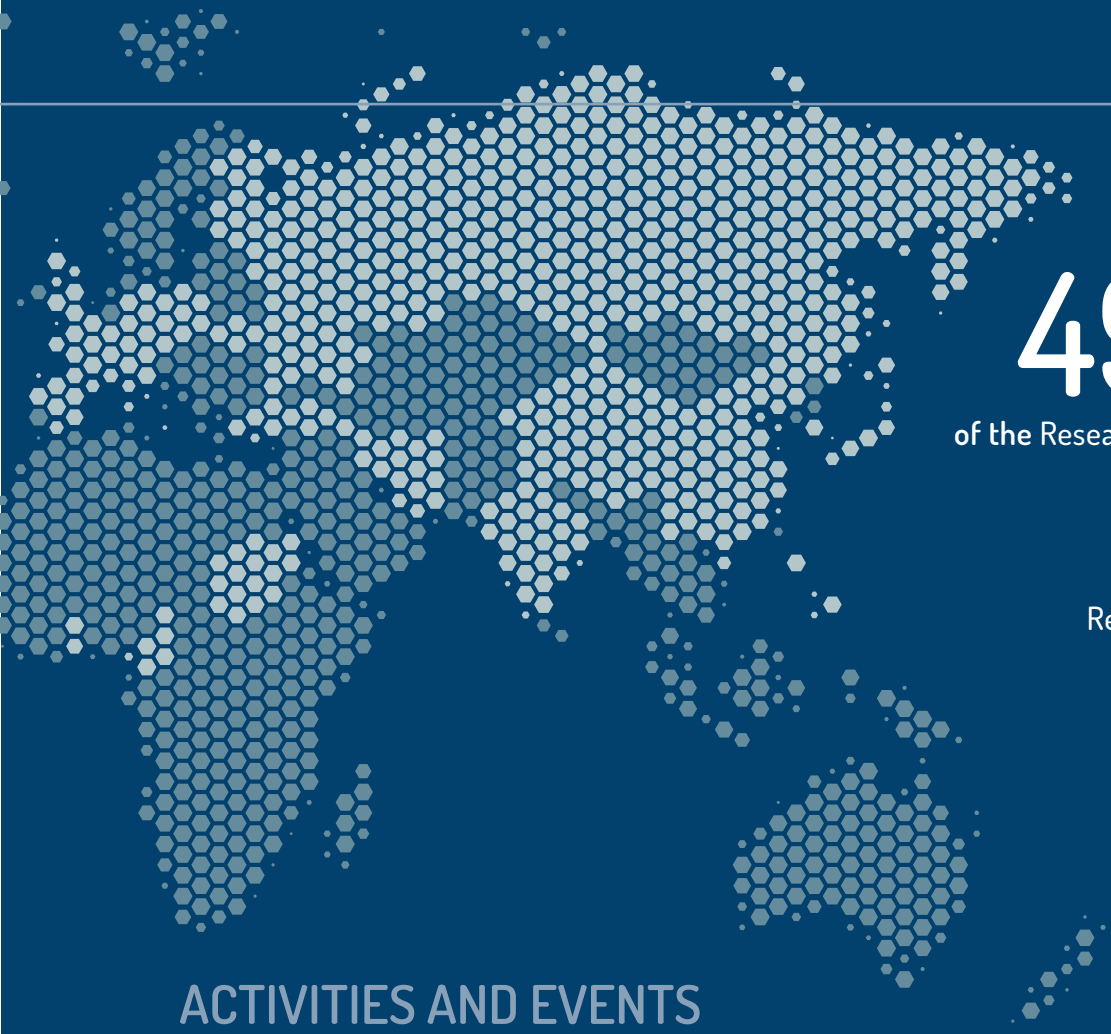
13 021

Q1 Publications[3]

69%

D1 Publications

43%



49%
of the Research Community is international

Researchers from
36
countries

ACTIVITIES AND EVENTS

Seminars
14

Conferences, Workshops and Courses[4]
3

Science and Society
28 Activities
10 000 Atendees

PROJECTS AND FUNDING

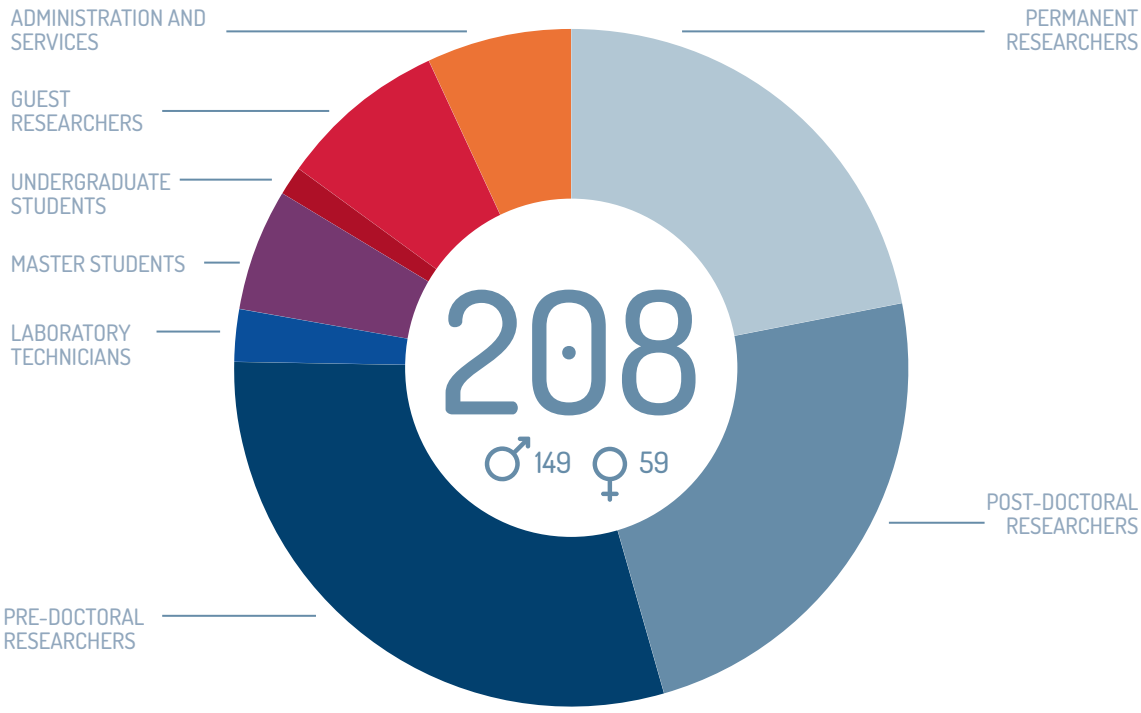
Ongoing Projects
82

Funding
5 088 818,50 €

[1] In the framework of the nanoscience master or supervised by CFM staff
[2] Including Physical Review B: 81%
[3] Source: Web of Science Core Collection as of April 2021
[4] Due to the pandemic, 6 events scheduled in 2020 had to be cancelled.

PEOPLE

ALL THE CFM COMMUNITY



CFM Staff

181

Researchers in Action

194 [3]

Permanent Researchers	46
Post-doctoral Researchers	49
Pre-doctoral Researchers	62
Laboratory Technicians	5
Master students[1]	12
Undergraduate students[2]	3
Guest Researchers	17
Administration and Services	14
Total	208

[1] Four of those receive scholarships during their stay at CFM and are considered staff

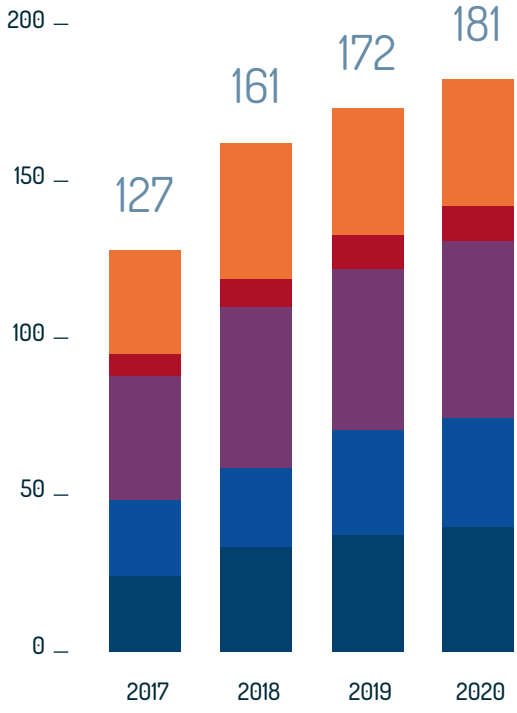
[2] One of those receive scholarships during their stay at CFM and is considered staff

[3] Including Guest researchers, undergraduate and master students

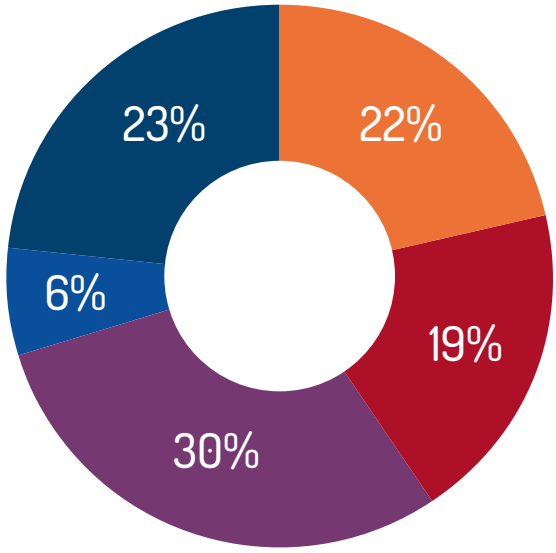
DISTRIBUTION OF CFM STAFF
according to the origin of their financial support

	2017	2018	2019	**2020**
CSIC	24	33	37	**40**
UPV/EHU	24	25	33	**34**
MPC-BERC	39	51	51	**56**
IKERBASQUE	7	9	11	**11**
COLLABORATORS	33	43	40	**40**
Total	127	161	172	**181**

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 2020



DIRECTION BOARD

Director: Daniel Sánchez Portal

General Manager: Amaia González Azpeitia

Before September 2020

Vicedirector: Andrés Arnau Pino

From September 2020

Vicedirector: Iñaki Juaristi Oliden

ADMINISTRATION AND SERVICES

Administration

Adolfo del Arco García, Administrative, CSIC

Amaia Gonzalez Azpeitia, Administration Manager, CSIC

Ane Iturriza Semperena, Administrative, MPC

Arantza Iturrioz Ezeiza, Project and Technology Transfer Manager, MPC

Elixabet Sarasketa Zabala, Project and Technology Transfer Manager, MPC

Idoia Mugica Mendiola, Outreach Manager, MPC

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

Laura Martín Montañez, Outreach Internship, MPC

María Formoso Ferreiro, Administrative, MPC

Marta López Pérez, Administrative, MPC

Txema Ramos Fernandez, Administrative, CSIC

Computing and IT 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

RESEARCHERS

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, Research Scientist, CSIC

Post-doctoral Researchers

Alberto Pablo Sánchez Muzas
Raúl Bombín Escudero

Pre-doctoral Researchers

Alberto Rodríguez Fernández
Alfredo Serrano Jiménez
Auguste Tetenoire

Guest Researchers

Raidel Martín Barrios, Pre-doctoral Researcher
Steven Lindner, Pre-doctoral Researcher

02 Quantum Phenomena on Surfaces

Permanent Researcher

Nicolás Lorente Palacios, Research Scientist, CSIC

Ikerbasque Fellow

Deungjang Choi, MPC

Post-doctoral Researchers

Felix Mouhat
Roberto Robles Rodríguez
Vladimir Zobac

Pre-doctoral Researchers

Cristina Mier González
José Reina Gálvez

03 Nanophysics Lab

Permanent Researchers

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

Ramon y Cajal Researcher

Sara Barja Martínez

Post-doctoral Researchers

Andrew P. Weber
Djuro Bikaljevic
Jan Patrick Calupitan
Khadiza Ali
Laura Fernández Gómez-Recuero
Marco Gobbi (Ikerbasque fellow on leave at CIC nanoGUNE)
Maxim Ilin
Rishav Harsh
Tao Wang
Vahagn Mkhitaryan

Pre-doctoral Researchers

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

Guest Researchers

Lorena Glatthaar, Master Student
Naoya Sumi, Pre-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
Mikhail Otrokov

Pre-doctoral Researchers

Joseba Goikoetxea Perez
Masoud Mansouri

Guest Researchers

Carlos Corona García, Pre-doctoral Researcher
Emre Bölen, Pre-doctoral Researcher
Pavel Jelinek, Senior Scientist

05 Spectroscopy at Atomic Scale

Permanent Researcher

Lucia Vitali, Ikerbasque Professor, UPV/EHU

Post-doctoral Researchers

Ana Barragán Durán
Jie Hou

Pre-doctoral Researcher

Francisco Javier Manterola Marañon

06 Theoretical and Computational Chemistry

Permanent Researcher

Pedro Braña Coto, Research Scientist, CSIC

Research Line:

Electronic Properties at the Nanoscale

07 Electronic Excitations in Surfaces and Nanostructures

Permanent Researchers

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

Post-doctoral Researchers

Ilya Nechaev
Marta Z. Pelc

Pre-doctoral Researchers

Mikel Arruabarrena Larrarte
Raúl Guerrero Avilés

Guest Researcher

Jozef Janovec, Pre-doctoral Researcher

08 Quantum Theory of Materials

Permanent Researchers

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

Post-doctoral Researcher

Raffaello Bianco

Pre-doctoral Researchers

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

Guest Researcher

Lorenzo Monacelli, Pre-doctoral Researcher

09 Mesoscopic Physics

Permanent Researchers

F. Sebastián Bergeret Sbarbaro, Tenured Scientist, CSIC
Vitaly Golovach, Ikerbasque Associate, UPV/EHU

Post-doctoral Researcher

Stefan Ilic

Pre-doctoral Researchers

Alberto Hijano Mendizabal
Cristina Sanz Fernández
Mikel Rouco Martin
Xian-Peng Zhang

10 Nano-Bio Spectroscopy

Permanent Researcher

Ángel Rubio Secades, University Professor, UPV/EHU

11 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 Researcher

Cheol-Hwan Park, Senior Scientist

12 Ceramic and Cement-Based Materials

Permanent Researcher

Jorge Sánchez-Dolado, Tenured Scientist, CSIC

Post-doctoral Researcher

Guido Goracci

Pre-doctoral Researcher

Mohammad Rahjoo

Guest Researchers

Mohammadreza Izadifar, Pre-doctoral Researcher
Valentina Musumeci, Pre-doctoral Researcher

Research Line:

Photonics

13 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
Rubén Esteban Llorente, Tenured Scientist, CSIC

Post-doctoral Researchers

Edurne Gorraitz Eusa
Mario Zapata Herrera
Luca Bergamini
Roberto Álvarez Boto

Pre-doctoral Researchers

Adrián Juan Delgado
Alvaro Nodar Villa
Antton Babaze Aizpurua
Bruno Candelas Peñalba
Carlos Maciel Escudero
Jonathan Antonio Sepúlveda Henríquez

Guest Researchers

Marvin Martin Müller, Pre-doctoral Researcher
Nahia Fagoaga Moreno, Master Student
Thomas Dutkiewicz, Master Student

14 Nanomaterials and Spectroscopy

Permanent Researchers

Yuri Rakovich, Ikerbasque Professor, UPV/EHU
Marek Grzelczak, Research Scientist, CSIC

Post-doctoral Researchers

María Sanromán Iglesias
Thomas Hendel

Pre-doctoral Researchers

Alba María Jumbo Nogales
Joscha Kruse
Sara Luisa Marina Barbier

Guest Researcher

Aimar Marauri Iriberri, Undergraduate Student

15 Laser Physics and Photonic Materials

Permanent Researcher

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

16 Quantum Nanophotonics Laboratory

Permanent Researcher

Gabriel Molina Terriza, Ikerbasque Professor, MPC

Post-doctoral Researchers

Francesc Monrabal Capilla
Juan José Miguel Varga
Rubén González Moreno

Pre-doctoral Researchers

Iker Gómez Viloria
Jon Lasa Alonso
Martin Molezuelas Ferreras

Master Student

Harriet Kumi

Research Line:

Polymers and Soft Matter

17 Polymers and Soft Matter

Permanent Researchers

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

Ikerbasque Fellows

Jon Maiz Sancho, MPC
Paula Malo de Molina Hernández, MPC

Post-doctoral Researchers

Beatriz Robles Hernández
Daniel Enrique Martínez Tong
Daniel José Arismendi Arrieta
José Ángel Martínez González
María Ester Verde Sesto
Mohammad Ali Aboudzadeh Barihi
Soheil Sharifi
Xabier Gaetan Monnier

Pre-doctoral Researchers

Agustín Blazquez Martín
Amaia Matanza Corro
Ane Izaskun Aranburu Leiva
Claudia Borredon
Davide Arena
Javier Martínez Sabando
Jokin Pinacho Olaciregui
Jordan Ochs
Jorge Humberto Melillo
Julen de la Cuesta Leone
Maiara Aime Iriarte Alonso
Mariarita Paciolla
Matteo Sanviti
Maud Formanek
Mohammed El Amine Hanifa
Numera Shafqat

Master Student

Jean Pierre Inchaustegui Revoredo

Undergraduate Student

Julen Olasagasti Imizcoz

Guest Researchers

Andrea Aguirre Baños, Master Student
Arianne Encinar Manzano, Master Student
Claudio Magnani, Master Student
Eric Gómez Urreizti, Undergraduate Student
Fernando Bresme, Senior Scientist
Jetro Epse Njukeng Nkengafac, Senior Scientist
Lucie Pavlaskova, Master Student
Timo Brändl, Post-doctoral Researcher
Virginia Vadillo Lacasa, Pre-doctoral Researcher

18 Quantum Beams and Sustainable Materials

Permanent Researcher

Felix Fernández Alonso, Ikerbasque Professor, MPC

Post-doctoral Researcher

Kacper Druzbicki

Pre-doctoral Researcher

Balthasar Braunewell

Guest Researcher

Mohammed Ali Al Assiri, Master Student

OTHER POSITIONS

Associate Professor

Isabel Tellería Echeverria, UPV/EHU

Senior Scientists

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

Post-doctoral Researchers

Wen Wan, DIPC (Miguel Moreno'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)
Pablo Herrero Gómez, DIPC (Dimas García de Oteyza's group)
Paul Lukas Dreher, DIPC (Miguel Moreno's group)

Master Students

Andrés Felipe Bejarano Sanchez, MPC / DIPC
Nathaniel Andrés Capote Robayna, MPC / DIPC

Guest Researcher

Jan Holec, Post-doctoral Researcher (Dimas García de Oteyza'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.

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
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.

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

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 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
	06 Theoretical and Computational Chemistry	Theoretical
Electronic Properties at the Nanoscale	07 Electronic Excitations in Surfaces and Nanostructures	Theoretical
	08 Quantum Theory of Materials	Theoretical
	09 Mesoscopic Physics	Theoretical
	10 Nano-Bio Spectroscopy	Theoretical
	11 Souza Research Group	Theoretical
	12 Ceramic and Cement-Based Materials	Experimental
Photonics	13 Theory of Nanophotonics	Theoretical
	14 Nanomaterials and Spectroscopy	Experimental
	15 Laser Physics and Photonic Materials	Experimental
	16 Quantum Nanophotonics Laboratory	Experimental
Polymers and Soft Matter	17 Polymers and Soft Matter	Theoretical and Experimental
	18 Quantum Beams and Sustainable Materials	Theoretical and Experimental

Sixteen 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*** (UPV/EHU) research building, in the ***Ibaeta*** Campus in Donostia / San Sebastián.

In 2020, Pedro Braña Coto, Research Scientist of CSIC, joined the staff of CFM. Together with Felix Fernández Alonso, Ikerbasque Professor at CFM since 2019, both of them have consolidated two new groups this year, "06 Theoretical and Computational Chemistry" and "18 Quantum Beams and Sustainable Materials", to reinforce the ***Chemical Physics of Complex Materials*** and ***Polymers and Soft Matter*** research lines respectively.

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.

Six research groups are included in this research line, with a high degree of complementarity. Four of the groups devote their activity to the ab-initio theoretical study of electronic structure and dynamical processes of nanostructures and molecules, 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), the "Modelisation and Simulation" group (04), and the "Theoretical and Computational Chemistry" group (06).

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 six research groups included in this research line are described.

1

Gas/Solid Interfaces

Group Leader: Ricardo Díez Muiño, Research Scientist, CSIC

The "Gas/Solid Interfaces" group focuses on the atomic-level understanding of physical and chemical processes arising at the interface between gas and solid phases of matter. The understanding of these elementary reactive and non-reactive processes is crucial in many energy- and environmental-related applications, including heterogeneous catalysis, electrochemistry, hydrogen storage, and fusion reactors.

The activity of the "Gas/Solid Interfaces" group relies on the development of new methodologies as well as on the use of first-principles electronic structure calculations to describe the interaction dynamics in such complex systems. Particular attention is paid to the development of theoretical models able to describe the non-adiabatic contributions and the energy dissipation channels that come into play, because they can drastically change the output of the dynamics.

Current research in the group also includes methodological advance in the simulation and analysis of photo-induced adsorbate dynamics and reactions, as well as the use of machine learning strategies specifically adapted to study the gas/solid interface dynamics.

2

Quantum Phenomena on Surfaces

Group Leader: Nicolás Lorente Palacios, Research Scientist, 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, with Dr. Deung-Jang Choi leading the experimental work and Dr. Nicolas Lorente leading the theoretical work. 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.

3

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, distributed in five different laboratory rooms.

4

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, particularly those based on graphene derivatives, (ii) to study the optical properties of complex organic/inorganic interfaces, (iii) to study the magnetic properties of different nanostructures, ranging from one dimensional systems to coordination networks and multilayer heterostructures 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 Autonomous Community.

5

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.

6

Theoretical and Computational Chemistry

Group Leader: Pedro Braña Coto, Research Scientist, CSIC

The group's research is focused on the theoretical investigation of excited state reactivity and dynamics in complex molecular systems. Researchers at this group use theory and simulation to characterize fundamental aspects of the photophysics and photochemistry of these systems with emphasis on charge and energy transfer and transport processes in novel materials with applications to nanoelectronics, organic photovoltaics, and lighting.

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 way to change their properties.

Six 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 as well as, the development of experimental characterization and design of cement based materials. The list of activities developed by the different groups follows:

7

Electronic Excitations in Surfaces and Nanostructures

Group Leader: Andrés Ayuela Fernández, Research Scientist, 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.

8

Quantum Theory of Materials

Group Leader: Ion Errea Lope, Associated 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.

9

Mesoscopic Physics

Group Leader: F. Sebastián Bergeret Sbarbaro, Research Scientist, CSIC

The "Mesoscopic Physics" group activity focuses on the theoretical aspects of quantum transport in nanostructures and mesoscopic systems. The main research covers various materials and structures, including metals, ferromagnets, semiconductors, superconductors, low dimensional systems, and topological matter. In addition to the theoretical activity, the group has a large network of experimental collaborators.

In the past years, particular emphasis is placed on the following research objectives: (i) to develop theoretical tools for studying spin-dependent transport in hybrid systems with spin-orbit coupling, exchange fields, and superconductivity; (ii) to analyze the electronic heat transport at the nanoscale; (ii) to explore the possibility of using superconducting materials for sensing and detection; and (iv) to design electronic and spintronics devices with new functionalities.

10

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 the 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 these topics include new developments within the many-body theory and TDDFT, covering ab-initio descriptions 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).

11

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 fields, 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.

12

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 CO_2 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 technologies in hydrothermal and supercritical fluids (SCF) 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 derived from cement-based materials, including both chemical storage (batteries) and thermal storage systems (TES) applications.

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.

13

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 an electron gas in nanostructures, the so-called surface 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 scanning 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, (vii) characterization of the dynamics and the coupling of emitters to be used in quantum information technology, and (viii) address non-linearities and collective effects in molecular optomechanics.

14

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.

15

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.

16

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 forces 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.

POLYMERS AND SOFT MATTER

The research line *Polymers and Soft Matter* focuses on the experimental and theoretical study of the structure and dynamics of complex molecular systems with an emphasis on polymers, soft matter and functional materials. Recently the "Quantum Beams and Sustainable Materials" group (18) was added to this research line, expanding the field of research and expertise on this area.

17

Polymers and Soft Matter

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

The general scientific objective of the activity program of this group is to achieve a fundamental understanding of the interplay between structure and dynamics at different length and time scales (micro, nano, meso, macro) in materials of increasing complexity based on polymers, glass-forming liquids and soft matter, in particular: polymers with different architectures, single-chain polymer nano-particles, multi-component, nano-structured and biopolymer systems. These materials exhibit complex dynamics and rheology and, in many cases, show hierarchical relaxations over many different length- and time-scales, which need to be unraveled. This in turn affects the processing and properties of the final materials. In order to rationally design appropriate materials and processes for various technological applications, a rigorous knowledge of the interplay between structure and dynamics at different length and time scales is demanded.

Taking inspirations from classical polymer physics, soft matter physics and the physics of condensed matter, over last years the "Polymers and Soft Matter" group has developed a robust and pioneering methodology to carry on this program. This methodology is based on the combination of different experimental relaxation techniques with neutron, XR and light scattering methods, molecular dynamics simulations and chemical synthesis oriented to polymers. The organization of the group is in fact driven by this methodology and the staff of the group (scientists belonging to the CSIC, the UPV/EHU and Ikerbasque) is composed by experts in different techniques/methods, all of them being involved in the scientific objectives defined at any time.

18

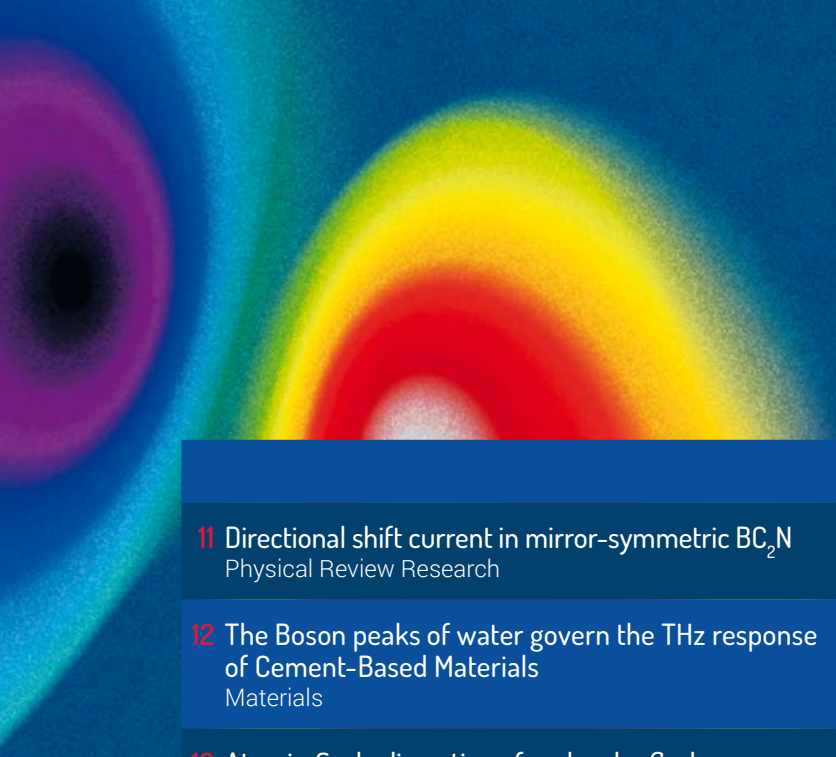
Quantum Beams and Sustainable Materials

Group Leader: Félix Fernández Alonso, Ikerbasque Professor, MPC

The "Quantum Beams and Sustainable Materials" group makes extensive use of beams of quantum particles like neutrons or photons in tandem with computational materials modelling to interrogate, understand, and design novel functional materials for energy applications and sustainability. This research program is underpinned by the development of new techniques and methodologies for materials discovery, in close collaboration with leading neutron and X-ray laboratories from around the globe.

Current areas of focus include hybrid organic-inorganic materials for photovoltaics & photonics, or carbon-based nanostructured media for the storage of chemical and thermal energy.

HIGHLIGHTS



		CFM GROUPS INVOLVED	PAGE
11	Directional shift current in mirror-symmetric BC_2N Physical Review Research	Souza Research Group	56
12	The Boson peaks of water govern the THz response of Cement-Based Materials Materials	Ceramic and Cement-Based Materials	57
13	Atomic-Scale dissection of molecular flashes Nature Nanotechnology	Theory of Nanophotonics	58
14	Strongly coupled exciton-plasmon nanohybrids reveal extraordinary resistance to harsh environmental stressors: temperature, pH and irradiation Nanoscale	Nanomaterials and Spectroscopy	59
15	Femtosecond laser direct inscription of 3D photonic devices in Er/Yb-doped oxyfluoride nano-glass ceramics Optical Materials Express	Laser Physics and Photonic Materials	61
16	Kerker conditions upon lossless, absorption, and optical gain regimes Physical Review Letters	Quantum Nanophotonics Laboratory	63
17	Coherent structural relaxation of water from meso- to inter-molecular scales measured using neutron spectroscopy with polarization analysis Physical Review Research	Polymers and Soft Matter	65
18	Direct observation of desorption of a melt of long polymer chains Nature Communications	Polymers and Soft Matter	67
19	Single-chain nanoparticles: opportunities provided by internal and external confinement Materials Horizons	Polymers and Soft Matter	69
20	The instrument suite of the European Spallation Source (ESS) Nuclear Instruments and Methods in Physics Research A	Quantum Beams and Sustainable Materials	71

1

Quantum corrections in the dynamics of hydrogen molecules at surfaces

Rodríguez-Fernández A, Bonnet L, Crespos C, Larregaray P, and Díez Muiño R.

Physical Chemistry Chemical Physics 22, 22805 (2020)

Static properties of surfaces are in general well known. Computational resources have become powerful enough to describe them using first principles and there is extensive output extracted from experimental measurements on their electronic, magnetic, and optical properties. Now, the challenge is the atomic- and molecular-level understanding of surface dynamics.

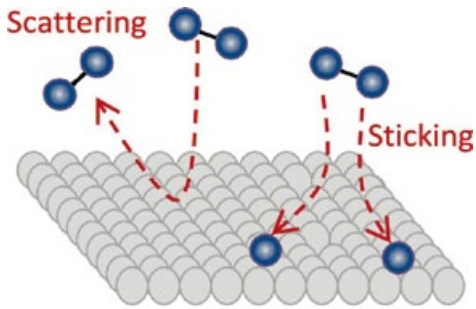
Elementary processes arising in gas/solid interfaces are ever-present in our daily life as well as in many industrial applications. The oxidation and corrosion of surfaces, the catalytic converters used in cars, the surface doping of semiconductors, or the industrial production of most synthetic compounds are all of them relevant examples of the importance of surface physical and chemical processes.

Synergetic advances in theory and molecular beam experiments associated with a tremendous increase of computing power have allowed a detailed understanding of the dynamics of chemical elementary processes. For gas phase reactions involving a small number of degrees-of-freedom, quantum dynamics calculations might be now regarded as exact because they generally provide results in excellent agreement with experiments. However, the complexity of surface reaction dynamics prevents an efficient and even effective use of quantum dynamics. A crucial issue is thus to develop accurate semiclassical tools able to make realistic predictions when major quantum effects come into play in the dynamics.

In this work, the authors improve over a classical trajectory method by including quantum corrections. The interaction between the molecules and the surface are described by density functional theory. They assign statistical weights to classical paths on the basis of two semiclassical corrections: Gaussian binning and the adiabaticity correction. This approach was previously applied by them to the heterogeneous gas–surface reaction between H_2 in its internal ground state and the Pd(111) surface [Rodríguez-Fernández et al., J. Phys. Chem. Lett., 2019, 10, 7629]. Its predictions of

the sticking and state-resolved reflection probabilities were found to be in surprisingly good agreement with those of exact quantum time-dependent calculations where standard quasi-classical trajectory calculations failed. This subsequent work shows that the quality of the calculations is kept when the incident H_2 molecules are rotationally excited, a feature extremely difficult to describe accurately.

"Within the Transborder Joint Laboratory QuantumChemPhys, CFM researchers and colleagues from the University of Bordeaux advance in the theoretical description of hydrogen sticking on metals."



High Accuracy of Quantum-Corrected Classical Simulations

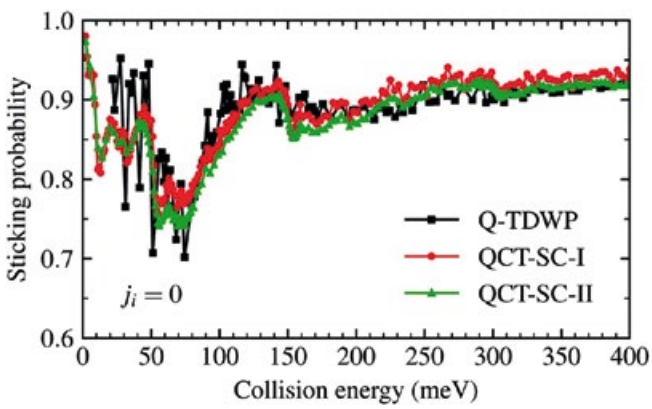


Figure: *Sticking probability for H_2 on Pd(111) as a function of the collision energy. Black symbols are purely quantum calculations. Red and green symbols represent quantum-corrected classical calculations.*

2

Vibron-assisted spin excitation in a magnetically anisotropic molecule

Bachellier N, Verlhac B, Garnier L, Zaldívar J, Rubio-Verdú C, Abufager P, Ormaza M, Choi DJ, Bocquet ML, Pascual JI, Lorente N, and Limot L.

Nature Communications 11, 1619 (2020)

The Scanning Tunneling Microscope (STM) drives electronic currents through a very small spatial region, allowing the excitation of single atoms and molecules. When an excitation is produced, the current increases because there are more transmission channels for the passing electrons. Then, by recording the current as a function of the applied bias between the tip of the STM and the surface, it is possible to obtain information on the molecule.

In this work, the authors use nickelocene molecules (see the figure a). This molecule is magnetic and anisotropic. This means that the molecular spin does not have complete symmetry. As a consequence, there are two degenerate excitations taking place at 3.8 meV and they correspond to turning the molecular spin by 90 degrees.

In the present work Bachellier et al. show that the molecule can also have vibrational excitations, and when the electrons have enough energy to simultaneously excite vibrational and spin degrees of freedom, they do it with an enormous efficiency. This is really surprising because inelastic electron transmission is usually thought to be less efficient than the corresponding elastic process, let alone to have two simultaneous excitations of the spin-excitation signal.

The authors have rationalized these findings in terms of the high efficiency of the spin excitation. It happens so likely that it is not deterred by the excitation of the vibration, leading to a very important spin+vibration signal. From the theory point of view, the results were equally puzzling. It was necessary to use a many-body formulation of the problem to be able to capture the excitation process. The model Hamiltonian contains electronic correlations that allow obtaining clear spin excitations by changing the electronic configuration. The surprise comes when an electron-vibration interaction is added to the Hamiltonian. Automatically the experimental result is recovered, not only opening the vibrational excitation, but also the vibrational and spin combined excitation. This is a surprise because there is no direct vibration-spin interaction in the Hamiltonian, but as in the experiment, the strong electron correlation suffices to create it.

"Electronic correlations give rise to very complex molecular excitations"

(a)

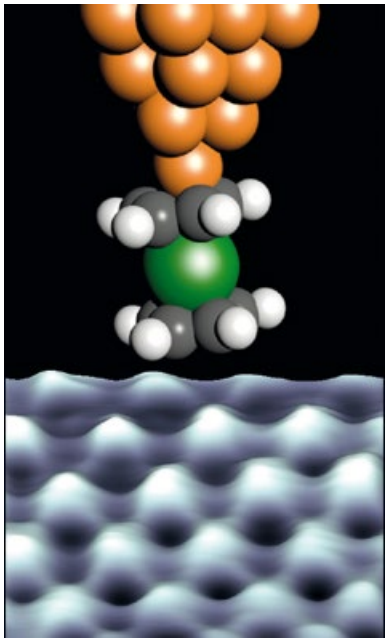
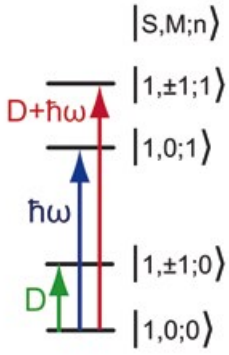
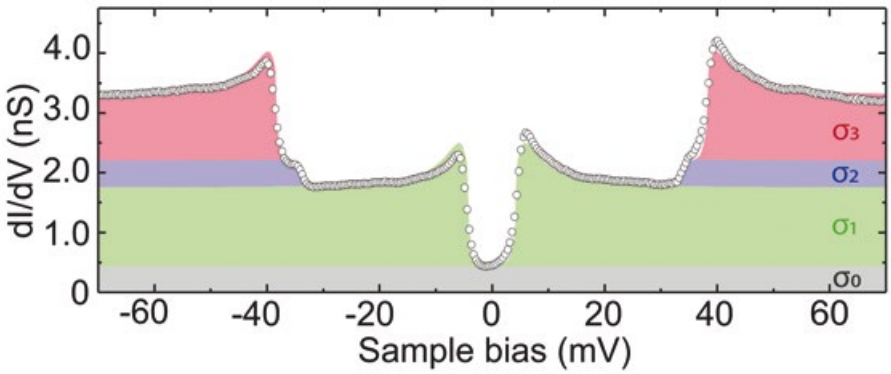


Figure: *(a) A nickelocene molecule ($C_{10}H_{10}$) trapped by an atom of the STM tip over a surface. (b) Energy levels with spin and vibrational degrees of freedom. D is the magnetic anisotropy equal to 3.8 meV and the frequency (ħω) is equal to 34 meV. (c) Differential conductance over the nickelocene adsorbates showing the first rapid increase at 3.8 mV, a second shoulder at 34 mV and the combined excitation at 38 mV.*

(b)



(c)



3

Simultaneous ignition of the CO oxidation at all facet planes of a curved platinum surface

Garcia-Martinez F, Garcia-Fernandez C, Simonovis JP, Hunt A, Walter A, Waluyo I, Bertram F, Merte LR, Shipilin M, Pfaff S, Blomberg S, Zetterberg J, Gustafson J, Lundgren E, Sanchez-Portal D, Schiller F, and Ortega JE.

Angewandte Chemie-International Edition 59, 20037 (2020)

CO oxidation ($2CO + O_2 \rightarrow CO_2$) on platinum metal surfaces is a model heterogeneous gas/surface catalytic reaction. Here, researchers investigated CO oxidation at different Pt crystal planes around the (111) direction, using a curved Pt surface. They surprisingly found that the ignition occurs simultaneously at all surface facets.

Platinum (Pt) is of upmost importance as a catalyst for car exhaust cleaning or for the water gas shift reaction, whereas Pt crystal surfaces are model systems for investigating the catalytic CO oxidation at the atomic scale. During decades, researchers have studied the sequential and simultaneous interaction of CO and O_2 with Pt under high vacuum conditions, providing a detailed description of fundamental steps in the reaction: O_2 dissociation, CO and O chemisorption, and CO-O interaction. Lately, a deeper insight is being gained through techniques operating at millibar pressures, such as Near Ambient Pressure X-ray Photoemission Spectroscopy (NAP-XPS). All these studies agree on the fundamental picture: the abrupt transition at "ignition", from the low-temperature poisoning stage, when CO covers the surface and blocks the reaction, to the high-temperature active stage, when CO is displaced from the surface by chemisorbed oxygen. However, the mechanism of such CO → O transition, and the differences among crystal planes, of enormous relevance in nanoparticle catalysis, remain unknown.

Researchers from the Nanophysics Lab of CFM, and Lund investigated the ignition of the CO oxidation reaction using a curved Pt surface (Figure a). Experiments combined Planar Laser Induced Fluorescence (PLIF) of CO (Lund, Figure b), with *operando* NAP-XPS (Brookhaven synchrotron, Figure c). PLIF images the ignition moment in the entire curved sample, showing that it occurs in all points simultaneously, irrespective of the reaction parameters. NAP-XPS identifies chemical species across the same surface at fixed temperature, providing the clues for this surprising behavior: as surface CO concentration decreases near ignition, minor amounts of O build up at the subsurface. DFT theory indicates that a CO-Pt-O complex develops that binds CO molecules to (111) terraces strongly, equaling CO adsorption energy in flat and stepped planes, and explaining why CO desorbs at the same temperature from all facets in the curved Pt surface.

"Researchers demonstrate that CO desorbs from flat and vicinal Pt surfaces at once, leading to a simultaneous CO oxidation reaction."

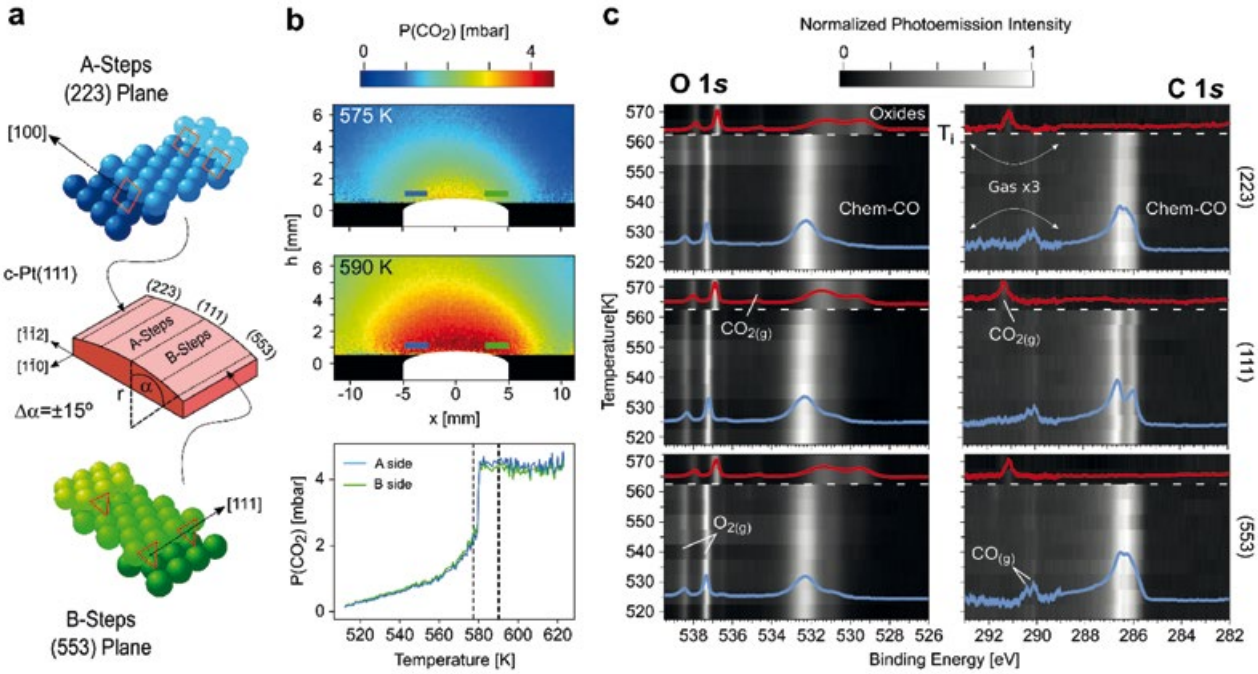


Figure: *Simultaneous ignition of the CO oxidation on a curved Pt surface. (a) Sketch of the c-Pt(111) curved crystal sample featuring A-type and B-type vicinal surfaces. (b) Top-middle, two-dimensional snapshots of Planar Laser Induced Fluorescence (PLIF) of CO_2 for a 6 mbar CO:O₂ mixture in front of the c-Pt(111) surface, right before (575 K) and after (590 K) light-off, illustrating the simultaneous ignition of the CO oxidation at all points. Bottom, CO_2 PLIF signal measured at the stepped A- and B-edges of the sample, marking the ignition at ~580 K. (c) O 1s (left) and C 1s (right) photoemission intensity images measured at three different points on the c-Pt(111) sample exposed to ~1 mbar CO:O₂ during a heating cycle. Vanishing of CO and emergence of oxygen-related species mark an abrupt, simultaneous ignition of the reaction.*

4

Strong interfacial exchange field induced by EuS ferromagnetic insulator measured in combination with heavy metals

Gomez-Perez JM, Zhang XP, Calavalle F, Ilyn M, Gonzalez-Orellana C, Gobbi M, Rogero C, Chuvilin A, Golovach VN, Hueso LE, Bergeret FS, and Casanova F.

Nano Letters 20, 6815 (2020)

Spin-dependent transport at heavy metal/magnetic insulator interfaces is the origin of many phenomena at the forefront of spintronics research. A characteristic feature of these heterostructures is the spin-dependent scattering of conduction electrons that gives rise to non-equilibrium but stationary states with non-uniform distribution of electrons with different spin orientations. Maintenance of this imbalance is achieved via dynamic separation of electrons and can be considered as a steady flux of spins (spin current). The concept of spin currents is widely used to describe many different phenomena such as spin pumping, spin Seebeck effect or spin Hall magnetoresistance. Furthermore, it is of key importance for the development of spin-torque – based devices such as magnetic random-access memory (STT-MRAM), currently ready for mass production.

Despite the importance of spin currents, there are not many heterostructures capable of generating this effect. Insulating magnetic materials (MI) are abundant, but the majority of them are ferri- or antiferromagnets, where the competing contributions from interfacial moments of opposite orientation complicate or cancel the net effect. Furthermore, archetypical insulating ferrimagnets like garnets have very complex crystal structures that complicate the growth of thin films with low density of defects, a crucial ingredient of high-quality heterostructures. For this reason, the development of a suitable technology for the growth of the ferromagnetic insulator EuS, accomplished by researchers of the Nanophysics Lab at CFM, is a crucial achievement.

Heterostructures of Pt/EuS were grown and patterned in Hall bars shape in collaboration with the Nanodevices

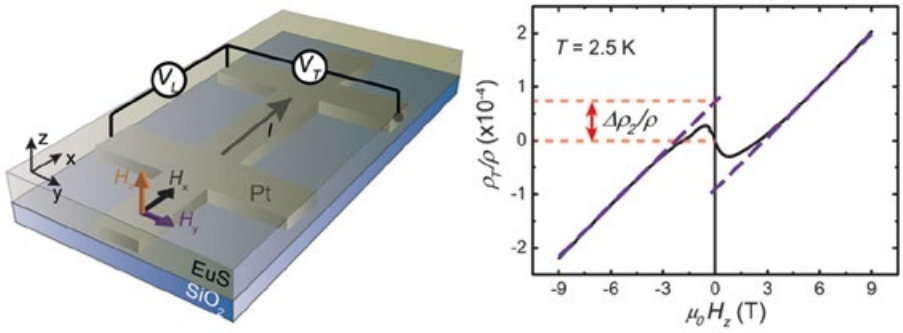


Figure: *Scheme of the fabricated Hall-bar devices and transverse resistivity measurement in Hall configuration. Dash purple lines correspond to the linear fit performed at large magnetic fields and extrapolated to zero. The red arrow shows the clear Δρ2/ρ.*

group at CIC nanoGUNE. Generation of spin current in these devices was studied via measuring of Spin Hall magnetoresistance (SMR) at low temperatures and in high magnetic fields. The theoretical model developed by researchers of the Mesoscopic Physics group at CFM allowed to quantify all three parameters defining the spin current through the interface: the spin-sink conductance Gs, which originates when the electron spins of the nonmagnetic metal are collinear with the MI magnetization and both the real and imaginary parts of the spin-mixing conductance G↑↓ = Gr + i*Gi, which originate from torques that the electron spins of the nonmagnetic metal exert to the magnetization of the MI when they are noncollinear. Gr is determined by the Slonczewski (or damping-like) torque, a quantity crucial for the spin–torque devices. On the other hand, Gi quantifies the exchange field between the electrons of the nonmagnetic metal and the magnetic moments of the MI, exerting a field-like torque when spin accumulation is induced. This interfacial exchange field is very relevant in different areas. For instance, when the nonmagnetic metal is a superconductor, it leads to a spin-splitting field, even in the absence of an external magnetic field.

A key finding of the work was a first time experimental demonstration that in ferromagnetic MI such as EuS, Gi is larger than Gr and at least 3 times larger at the lowest measured temperature (2.5K), as was predicted theoretically for europium chalcogenides. It was confirmed that the field-like torque plays an important role in Pt/EuS because all magnetic moments of the interface contribute to the interfacial exchange field, as opposed to the ferrimagnetic case, where there is a compensation of the magnetic moments.

5

Magnetism of topological boundary states induced by boron substitution in graphene nanoribbons

Friedrich N, Brandimarte P, Li J, Saito S, Yamaguchi S, Pozo I, Peña D, Frederiksen T, Garcia-Lekue A, Sánchez-Portal D, and Pascual JI.

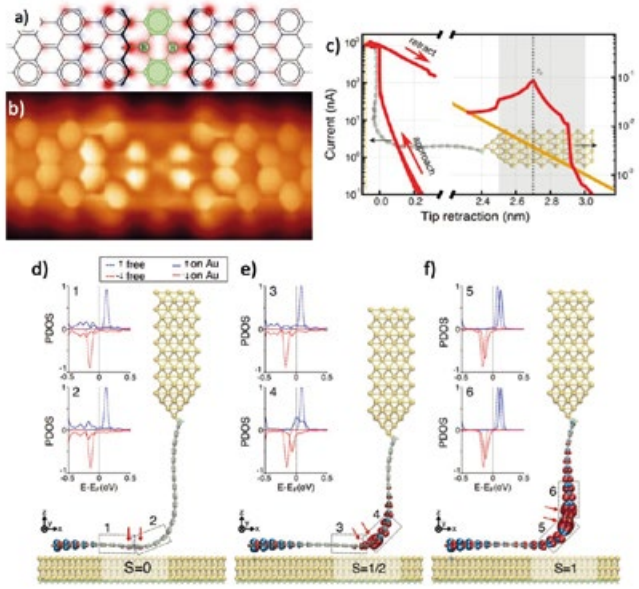
Physical Review Letters 125, 146801 (2020)

Graphene nanoribbons (GNRs), low-dimensional platforms for carbon-based electronics, show the promising perspective to also incorporate spin polarization in their conjugated electron system. However, these magnetic moments are usually localized around zigzag edges, difficult to fabricate and very reactive. This combined theoretical and experimental study demonstrates that magnetism can also be induced away from physical edges through atomically precise engineering of topological defects in its interior. A pair of substitutional boron atoms inserted in the carbon backbone breaks the conjugation of their topological bands and builds two spin-polarized boundary states around them.

GNRs can be classified according to the topology of their electronic band structures. This allows predicting the appearance of zero-energy states bound at the boundaries between GNRs of different topological classes or at the edges of topologically non-trivial ribbons. These localized states give rise to spin polarization once electron-electron repulsion is taken into account. Beyond an academic problem, this offers the promise of using topology to induce magnetism in carbon-based platforms. Unfortunately, the magnetism of topologically protected boundary states in carbon systems had yet to be demonstrated, while topological engineering of boundary states seems restricted to exotic cases, always involving the highly reactive zigzag edges.

The authors of this work show that magnetic boundary states can be created in the interior of a GNR simply by embedding substitutional heteroatoms in the carbon backbone. A pair of boron atoms substituting carbon turns out to act as a physical termination for the topological valence band of the ribbon (7-AGNR) and, hence, creates end states that are singly occupied and spin polarized. First indications of the presence of magnetism were given by the appearance of characteristic Kondo peaks in electrical transport experiments performed at CIC nanoGUNE. Transport was measured through boron-substituted GNRs suspended between the tip and the sample of a Scanning Tunneling Microscope (STM). These observations were rationalized in terms of the theory and first-principles simulations performed at CFM and DIPC, which predicted for each isolated boron pair a S=1 spin state as well as a strong dependence on the spacing between pairs. The interaction between two of such topological defects was further explored, outlining a route to engineer topological spin chains, with the promising tunability of their magnetism by modifying their spacing.

This work presents a remarkable combination of high precision electrical transport experiments of an atomically perfect system in a free-standing configuration between source/drain electrodes with atomistic simulations of the experimental configuration (involving a large number of atoms). These complex simulations were further used to develop and parametrize intuitive models governing the onset of magnetism in this system.



"These results demonstrate a route to embed spin chains in graphene nanoribbons, turning them into basic elements of spintronic devices"

Figure: *a) Structure of the 2B-7AGNR defect shown over a color map representing the computed spin polarization density map (green represents the boron moiety). b) Constant height STM scan (V=2 mV) using a CO-functionalized tip of a 2B-7AGNR defect. c) Tunneling current I at V=25 mV as a function of z for a borylated (red) and a pristine (orange) GNR, for comparison. Observe the large current increase around the point (z_p) at which the B-pair is detached from the substrate. (d)–(f) Relaxed structures of three different configurations of a 2B-7AGNR bridging a gold tip and a Au(111) surface (red arrows indicate the B atoms). Constant spin density isosurfaces are shown with spin up in blue and down in red. Insets compare spin PDOS over C atoms within the boxed regions around each boron atom for each bridge geometry (solid lines), with the corresponding one of a free 2B-7AGNR (dashed lines).*

6

Anisotropic electron conductance driven by reaction byproducts on a porous network of dibromobenzothiadiazole on Cu(110)

Barragan A, Sarasola A, and Vitali L.

Angewandte Chemie-International Edition 59, 15599 (2020)

Organic compounds offer a variety of functional properties eligible almost on demand. However, the application of organics into devices requires in addition excellent charge transport properties at energies larger than 2eV, where electronics works. Here, Barragan et al. show a mechanism enabling one-dimensional conductance-channels connecting discrete molecular states at 2.1eV through the pores of a metal-organic network on Cu(110).

In the last decade, a considerable scientific attention has been devoted to the formation of ordered organic structures ensuring molecular functionalities and good electrical properties. In this context, a valuable approach was offered by Ullmann cross-coupling reactions where halogenated molecules catalyzed by metal surfaces promoted the synthesis of extended structures through the molecular polymerization. This chemical approach results in good mechanical and electrical contacts between components. In this collaborative work between the Donostia International Physics Center (DIPC), the University of the Basque Country (UPV/EHU) and CFM, the authors show that the electron conductance of benzothiadiazole molecules, extensively used in electronics, can be enhanced even before their polymerization. Indeed, despite the formation of a porous network, two adjacent, periodic and isoenergetic contributions, namely a molecular electronic resonance and the confined surface-state, sum-up forming one-dimensional conductance channels, observable in energy-resolved maps of a 2D-metal-organic network. Though they do not contribute directly to the conductance, the adsorption configurations of Br atoms, inorganic byproduct of the redox-reacted 4,7-dibromobenzo[c]-1,2,5-thiadiazole molecules on the copper surface critically control the channel continuity. These halogen atoms enable the delocalization of the molecular electronic resonance into a continuous channel acting on the confinement of the Cu(110) surface state on the pores. Small displacements of the Br atoms change the local surface potential misaligning the energy levels and creating discontinuity into the channels. This work opens new perspectives on charge-transport mechanisms controlled by an order-disorder transition determined by the movement of single atoms limiting carrier's mobility in two-dimensional organic networks.

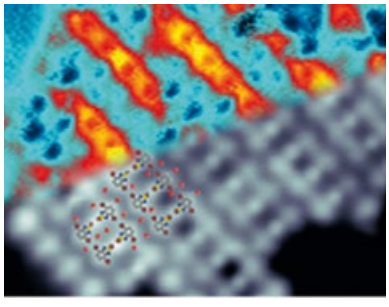


Figure: *Graphical representation of the conductance channels and the topographic structure that enables them. The molecular modeling of the 4,7-dibromobenzo[c]-1,2,5-thiadiazole (2Br-BTD) molecules on the copper surface is superposed: Br atoms are depicted as bright red dots in the sketch.*

7

Fabrication of a novel magnetic topological heterostructure and temperature evolution of its massive Dirac cone

Hirahara T, Otrokov MM, Sasaki TT, Sumida K, Tomohiro Y, Kusaka S, Okuyama Y, Ichinokura S, Kobayashi M, Takeda Y, Amemiya K, Shirasawa T, Ideta S, Miyamoto K, Tanaka K, Kuroda S, Okuda T, Hono K, Eremeev SV, and Chulkov EV.

Nature Communications 11, 4821 (2020)

Using Angle Resolved Photoemission Spectroscopy (ARPES) and ab initio calculations, Hirahara et al. have studied the molecular beam epitaxy grown heterostructure $Mn_4Bi_2Te_7$/Bi_2Te_3 achieved by self-organization of the Mn and Te adatoms co-deposited on Bi_2Te_3. The authors reveal a sizable Dirac point gap and study its temperature evolution.

Although the interfaces between trivial magnetic and topological nonmagnetic insulators have recently attracted a great deal of attention, no photoemission evidence of the Dirac point gap opening in the topological interface state has been reported. To bridge this gap, the authors have synthesized a novel magnetic topological heterostructure with a built-in interface achieved via self-organization of the MnTe film inside of the Bi_2Te_3 surface quintuple layer block (e.g., Te–Bi–Se–[MnTe]–Bi–Te), where the magnetic film has adopted its bulk-like (NiAs-like) structure, see Figure (a). The resulting structure can be written as $Mn_4Bi_2Te_7/Bi_2Te_3$. Strikingly, the realization of this scenario leads to a unique situation when the heterostructure's magnetic part is based on a material that intrinsically does not show Van der Waals bonding (MnTe), but turns out to be Van der Waals coupled to a topological insulator substrate.

ARPES measurements of $Mn_4Bi_2Te_7/Bi_2Te_3$ reveal a massive Dirac cone with a gap of 40-75 meV at 16 K (Figure b). The system showed long-range magnetic order with a critical temperature of about 20 K. *Ab initio* calculations predict a complicated magnetic configuration for $Mn_4Bi_2Te_7/Bi_2Te_3$ combining both ferromagnetic and antiferromagnetic couplings between adjacent layers (Figure c, inset). Surface electronic structure calculations confirm the existence of the gapped Dirac cone for these crystal and magnetic structures (Figure c). Further, by tracing the temperature evolution, they find the Dirac point gap to gradually decrease with increasing temperature, whith a transition from a massive to a massless Dirac cone occurring around 200–250 K. Thus, these results show for the first time that the Dirac

point gap of the interface topological state of the magnetic topological heterostructure eventually closes, albeit at a temperature well above the magnetic critical temperature. Such findings open a new direction in studies of the magnetic insulator/topological insulator interfaces and restore their potential for the observation of the quantum anomalous Hall and topological magnetoelectric effects.

"In this heterostructure, a non Van der Waals material connects in a Van der Waals fashion to a topological insulator, which makes the magnetic insulator/topological insulator interfaces good for observing the quantized topological effects"

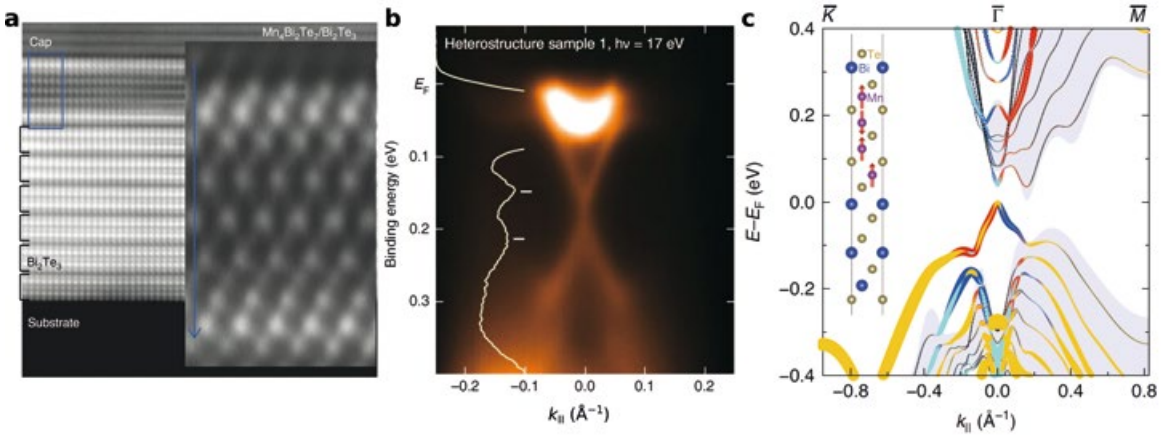


Figure: *(a) Scanning transmission electron microscope image of the $Mn_4Bi_2Te_7/Bi_2Te_3$ heterostructure measured at room temperature. The inset shows the atomically-resolved image. (b) Band dispersion of the heterostructure sample measured with ARPES. The white line shows the energy distribution curve at the Γ-point. (c) Calculated band dispersion of the $Mn_4Bi_2Te_7/Bi_2Te_3$ heterostructure. The inset shows the predicted magnetic structure.*

8

Quantum fluctuations sustain the record superconductor

Errea I, Belli F, Monacelli L, Sanna A, Koretsune T, Tadano T, Bianco R, Calandra M, Arita R, Mauri F, and Flores-Livas JA.

Nature 578, 66 (2020)

Reaching room-temperature superconductivity is one of the biggest dreams in physics. Its discovery would bring a technological revolution by providing electrical transport with no loss, ultra efficient electrical engines or generators, as well as the possibility of creating huge magnetic fields without cooling. The recent discoveries of superconductivity first at 200 kelvin in hydrogen sulfide and later at 250 kelvin in LaH_{10} have spurred attention to these materials, bringing hopes for reaching room temperatures soon. It is now clear that hydrogen-rich compounds can be high-temperature superconductors, at least at high pressures; both discoveries were made above 100 gigapascals, one million times atmospheric pressure.

The 250 kelvin (-23ºC) obtained in LaH_{10}, the usual temperature at which home freezers work, is the hottest temperature for which superconductivity has ever been observed. The possibility of high-temperature superconductivity in LaH_{10}, a superhydride formed by lanthanum and hydrogen, was anticipated by crystal structure predictions back in 2017. These calculations suggested that above 230 gigapascals a highly symmetric LaH_{10} compound (Fm-3m space group), with a hydrogen cage enclosing the lanthanum atoms (see figure), would be formed. It was calculated that this structure would distort at lower pressures, breaking the highly symmetric pattern. However, experiments performed in 2019 were able to synthesize the highly symmetric compound at much lower pressures, from 130 to 220 gigapascals, and to measure superconductivity around 250 kelvin in this pressure range. Therefore, the crystal structure of the record superconductor, and thus its superconductivity, remained not entirely clear.

Now, this work shows that atomic quantum fluctuations "glue" the symmetric structure of LaH_{10} in all the pressure range in which superconductivity has been observed. In more detail, the calculations show that if atoms are treated as classical particles, that is, as simple points in space, many distortions of the structure tend to lower the energy of the system. This means that the classical energy landscape is very complex, with many minima (see figure), like a highly deformed mattress because many people are standing on it. However, when atoms are treated like quantum objects, which are described with a delocalized wave function, the energy landscape is completely reshaped: only one minimum is evident (see figure), which corresponds to the highly symmetric Fm-3m structure.

Somehow, quantum effects get rid of everybody in the mattress but one person, who deforms the mattress only in one single point.

"This result suggests that superconductivity approaching room temperature may be possible in hydrogen-rich compounds at much lower pressures than previously expected with classical calculations."

Furthermore, the estimations of the critical temperature using the quantum energy landscape agree satisfactorily with the experimental evidence. This supports further the Fm-3m high-symmetry structure as responsible for the superconducting record.

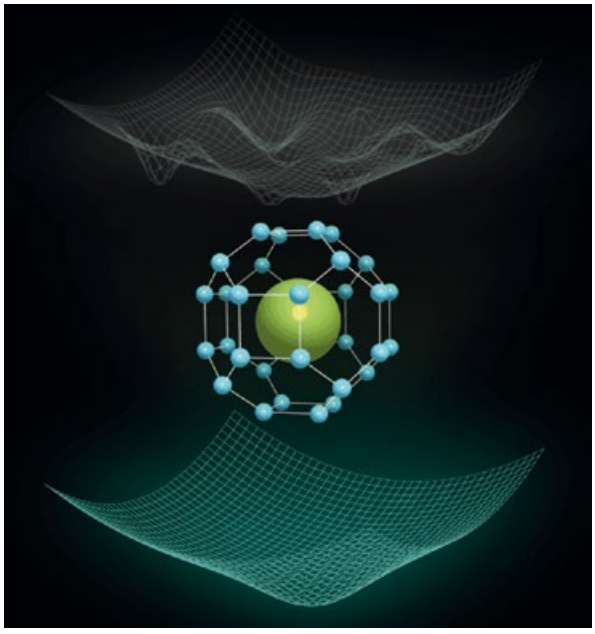


Figure: *Crystal structure of the Fm-3m phase of LaH_{10}, where a highly symmetric hydrogen cage encloses the lanthanum atoms. In the top a sketch of the complex classical energy landscape is shown, where many minima are present. On the other hand, in the bottom the image shows a sketch of the completely reshaped much simpler quantum energy landscape, where only one minimum survives.*

9

A Josephson phase battery

Strambini E, Iorio A, Durante O, Citro R, Sanz-Fernandez C, Guarcello C, Tokatly IV, Braggio A, Rocci M, Ligato N, Zannier V, Sorba L, Bergeret FS, and Giazotto F.

Nature Nanotechnology 15, 656 (2020)

Strambini et al. demonstrate a quantum device that provides a persistent phase bias to a superconducting circuit. It consists of a InAs nanowire proximitized by Al superconducting leads. The ferromagnetic polarization of the unpaired-spin states is efficiently converted into a persistent phase bias across the wire. The observed symmetries in the magnetic field confirm the predictions of the theoretical model previously presented by the authors.

A classical battery converts chemical energy into a persistent voltage bias that can power electronic circuits. We denote a phase battery as a quantum device that provides a persistent phase bias to a quantum circuit's wave function. It represents a key element for quantum technologies based on phase coherence. In the present work, the authors demonstrate the first implementation of a phase battery in a hybrid superconducting circuit.

The device is shown in figure (a). It consists of an n-doped InAs nanowire (red) with unpaired-spin surface states, proximitized by Al superconducting leads (blue). The authors found that the ferromagnetic polarization of the unpaired-spin states is efficiently converted into a persistent phase bias φ_0 across the wire, leading to the anomalous Josephson effect. The phase bias can be controlled by an external magnetic field [figure (b)], achieving a continuous tuning of φ_0 [figure (c)]. Hence, it is possible to charge and discharge the quantum phase battery. The observed symmetries of the anomalous Josephson effect in the vectorial magnetic field agree with the theoretical predictions calculated by the authors [figure (d)] in a previous work[1,2].

"Predictions done by the Mesoscopic Physics group at CFM on spontaneous currents in systems with strong spin-orbit coupling have been experimentally verified in this collaboration"

[1] Bergeret FS, and Tokatly IV
Theory of diffusive φ_0 Josephson junctions in the presence of spin-orbit coupling.
EPL 110, 57005 (2015).

[2] Konschelle F, Tokatly IV, and Bergeret FS
Theory of the spin-galvanic effect and the anomalous phase shift φ_0 in superconductors and Josephson junctions with intrinsic spin-orbit coupling
Physical Review B 92, 125443 (2015).

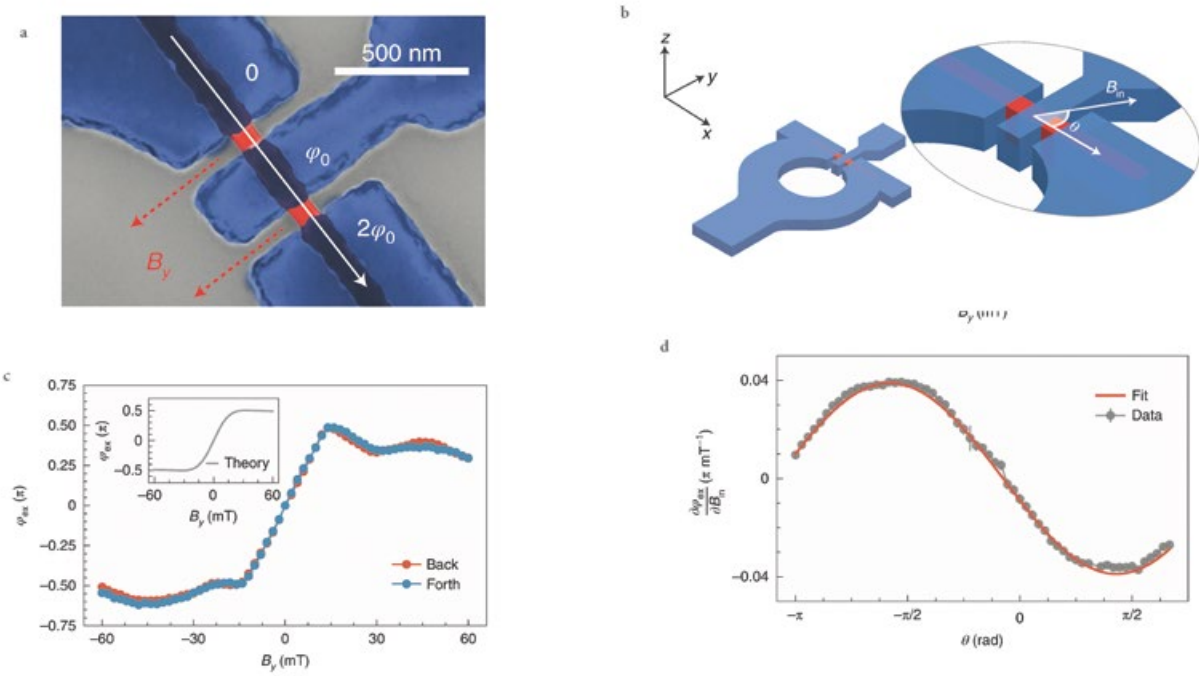


Figure: *(a) Scanning electron microscopy image of the active region of the phase battery composed by the two φ_0-junctions. B_y is the in-plane magnetic field orthogonal to the nanowire. (b) Sketch of the interferometer with the reference axes of the in-plane magnetic field (Bin) and the angle θ with respect to the nanowire axis. (c) Dependence of the extrinsic anomalous phase φex on B_y. It results in an odd symmetry and non-hysteretic back and forth sweeps (blue and red traces). Inset: the φex(B_y) dependence obtained from our theoretical model. (d) Plot of ∂φex/∂Bin versus θ together with a theoretical fit (red curve).*

These results demonstrate how the combined action of spin-orbit coupling and exchange interaction induces a strong coupling between charge, spin, and superconducting phase, able to break the phase rigidity of the system. This quantum element, providing a controllable and localized phase bias, can find applications in different quantum circuits, such as an energy tuner for superconducting flux and hybrid qubits, or a persistent multi-valued phase-shifter for superconducting quantum memories as well as superconducting rectifiers. Moreover, the magnetic control over the superconducting phase opens new avenues for advanced schemes of topological superconducting electronics based on InAs junctions.

10

Twisted 2D material gives new insights into strongly correlated 1D physics

Kennes DM, Xian L, Claassen M, and Rubio A.

Nature Communications 11, 1124 (2020)

Researchers from the Max Planck Institute for the Structure and Dynamics of Matter (MPSD) in Hamburg, the RWTH Aachen University (both in Germany), the Flatiron Institute in the USA, and CFM have revealed that the possibilities created by stacking two sheets of atomically thin material atop each other at a twist are even greater than expected.

The four scientists examined germanium selenide (GeSe), a material with a rectangular unit cell, rather than focusing on lattices with three- or six-fold symmetries like graphene or WSe_2. By combining large scale ab-initio and density matrix renormalization group calculations, the researchers showed that the Moiré interference pattern creates parallel wires of correlated one-dimensional systems.

This considerably broadens the scope for realizable structures using Moiré twisting physics and provides an inroad into the challenging question of how a correlated system crosses over from two dimensions to one. Because the particles cannot pass each other as they would in a multi-dimensional context, one-dimensional systems are intriguing, as correlations necessarily lead to collective excitations.

Dante Kennes says the combined analysis of the two numerical methods yielded great results: "We were able to classify the phase diagram of two sheets of twisted GeSe and found a plethora of realizable phases of matter, including correlated Mott insulators and the so-called Luttinger liquid phase, which reveals physics defying our independent particle picture in fundamental ways. "Lede Xian adds: "We established twisted GeSe as an exciting platform to understand strongly correlated 1D physics and the crossover from one to two dimensions in a highly tunable and experimentally accessible manner."

"The present work provides valuable insights into how twisting 2D materials can be used to create properties on demand in quantum materials"

This research opens up many future directions. One particularly intriguing approach is to substitute elements in GeSe to achieve higher spin-orbit coupling. Martin Claassen from the Center for Computational Quantum Physics at the Flatiron Institute points out: "Coupling such a system to a superconducting substrate would result in topologically protected Majorana edge modes under the right conditions". Those states are particularly important as they could be used as so-called qubits; the quantum equivalent of a classical bit, which is the fundamental computational building block.

Therefore, the ability to create many parallel Moiré wires with Majoranas attached at their ends reveals an intriguing future inroad for unlocking topological quantum computing in a naturally scalable way. Ángel Rubio, the director of the MPSD's Theory department, concludes: "The present work provides valuable insights into how twisting 2D materials can be used to create properties on demand in quantum materials".

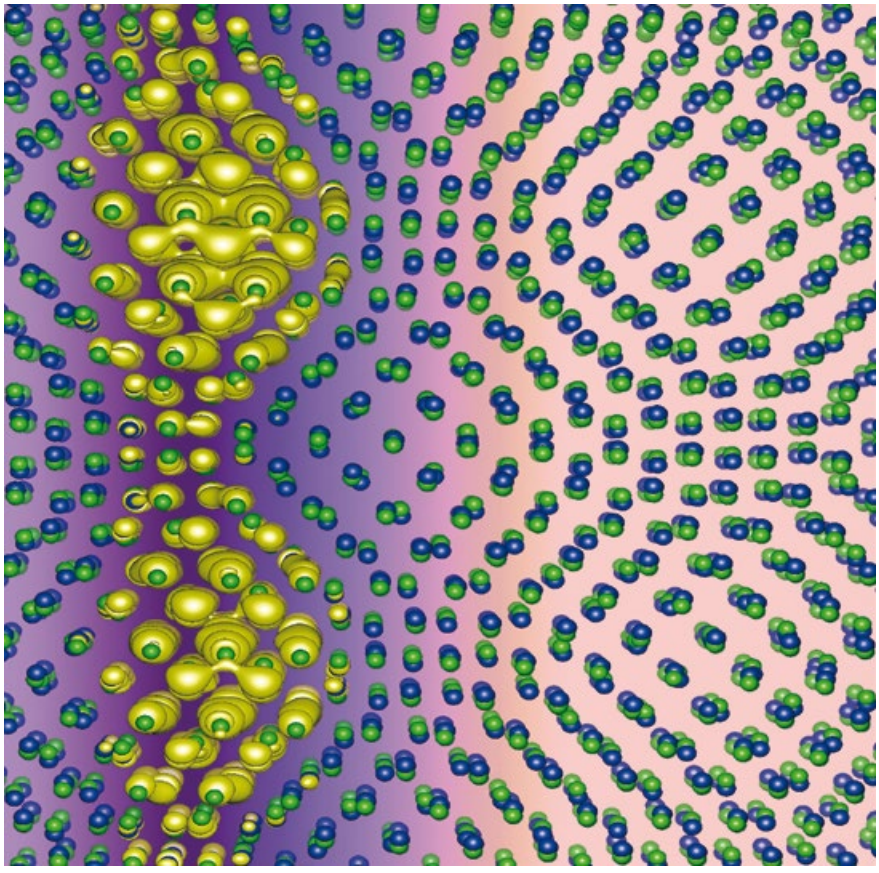


Figure: *One-dimensional correlated states emerge in twisted bilayer germanium selenide. The figure shows the charge density distribution of such states obtained from density function theory calculations. © Lede Xian, Jörg Harms, MPSD*

11

Directional shift current in mirror-symmetric BC_2N

Ibanez-Azpiroz J, Souza I, and De Juan F.

Physical Review Research 2, 13263 (2020)

Ibanez-Azpiroz et al. theoretically describe the shift-current photoconductivity of graphitic BC_2N. It is strongly anisotropic near the fundamental gap due to quantum dipole selection rules imposed by mirror symmetry, which imply that the relative parities between valence and conduction bands are key for determining the directionality of the band-edge response.

Quick, manipulable and efficient conversion of light into electricity is key for future clean-energy technologies. The bulk photovoltaic effect, also known as the shift current, is a nonlinear absorption process that converts light into electrical current intrinsically, and has attracted increased attention in recent years due to potential applications in solar cells.

In this work, the authors report a distinctive shift-current response at the band-edge of a noncentrosymmetric polytype of graphitic BC_2N, a quasi two dimensional layered semiconductor made of alternating zigzag chains of carbon and boron nitride. They perform accurate density functional theory calculations of the shift photoconductivity employing a recently developed formalism based on Wannier interpolation.

The group's *ab initio* calculations show that near the fundamental band gap the calculated response exhibits strong anisotropy, due to the vanishing of certain tensor components not foretold by phenomenological symmetry arguments. They trace the origin of this anisotropy to the mirror symmetry of the crystal, which imposes quantum selection rules on dipole transitions between the valence and conduction bands near the fundamental band gap. In addition to the density functional theory analysis, the researchers also capture the essential physics of this phenomenon with a two-band $k \cdot p$ model, thus providing a suitable framework for a broad class of materials.

"Dipole selection rules determine the nonlinear response to light of graphitic BC_2N"

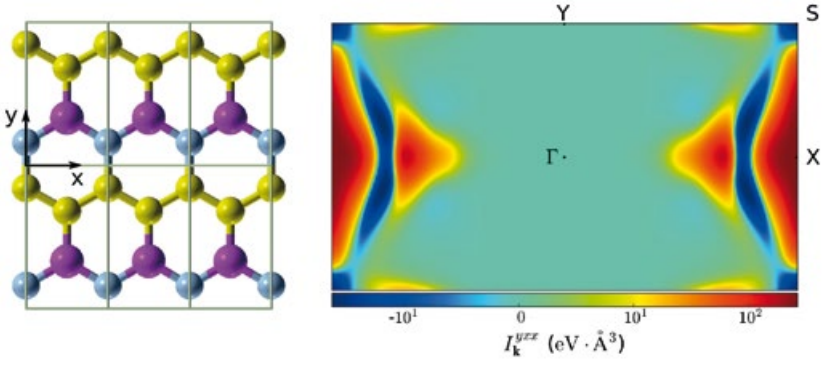


Figure: *(Left) Crystal structure of one layer of BC_2N, where magenta, grey and yellow balls represent boron, nitrogen and carbon atoms, respectively. (Right) Heatmap plot across the 2D Brillouin zone at $k_z = 0$ of the yx matrix element of the shift photoconductivity.*

12

The Boson peaks of water govern the THz response of cement-based materials

Dolado JS, Goracci G, Duque E, Martauz P, Zuo YB, and Ye G.

Materials 13, 4194 (2020)

To find materials with an appropriate response to THz radiation is key for the incoming THz technology revolution. Unfortunately, this region of the electromagnetic spectra remains largely unexplored in most materials. In particular, ubiquitous and cheap materials like cementitious materials deserve due attention.

Cementitious materials contain many structural features that seem to favour the response to the THz radiation. On the one hand, their local structure is glassy and amorphous, something which is known to give rise to an overpopulation of vibrational states at the THz frequencies, the so-called Boson Peaks. On the other hand, they contain plenty of water molecules that strongly interact with light due to their intrinsic electric dipole. Besides, the nanoporous skeleton of cement-based materials provides a rich topology for investigating the intrinsic Bosonic states of water, often studied in supercooled or nanoconfined water.

In this work, researchers from the CFM, in collaboration with researchers from the TU Delft (Netherlands), Povazska Cementaren (Slovakia) and Huazhong University of Science and Technology (China), have identified the THz fingerprints of cement-based materials. To this end, THz transmission experiments have been carried out over cement pastes in combination with atomistic simulations. Interestingly both the experiments and simulations have revealed that cementitious materials exhibit three main peaks at frequencies around ~0.6 THz, ~1.05 THz and ~1.35 THz, which are related to the Bosonic states of their water content. Additionally, two extra signals appear at ~1.95 THz and ~2.75 THz, coming from modes of the floppy parts of the dried skeleton.

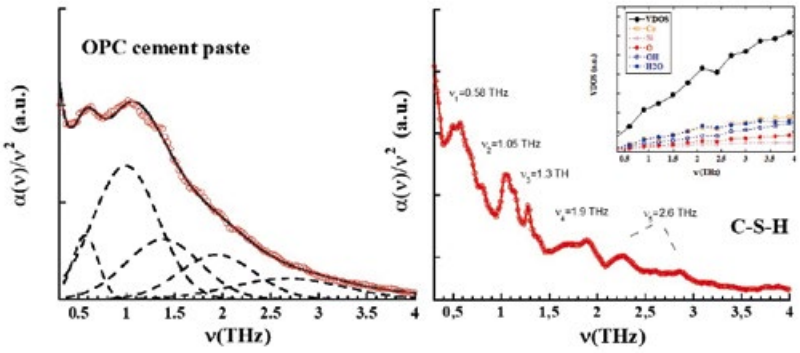


Figure: *(a) Experimental absorbance of the Ordinary Portland Cements (OPC) cement paste, together with the deconvolution of the spectra. (b) Computational prediction of the absorbance of C-S-H gel (the most important ingredient of cementitious materials). In the inset the Vibrational Density of States (VDOS) and their projections are displayed.*

13

Atomic-scale dissection of molecular flashes

Doppagne B, Neuman T, Soria-Martinez R, Lopez LEP, Bulou H, Romeo M, Berciaud S, Scheurer F, Aizpurua J, and Schull G.

Nature Nanotechnology 15, 207 (2020)

Molecules are key building blocks for future optoelectronic devices at extremely low dimensions, as they can carry electronic current, emit photons, or switch on and off a signal. Thanks to an ultra-resolved nanoscopy technique, it is now possible to map the origin of light emitted from a switching molecule with intramolecular resolution.

Single-molecule devices open up functionalities that go beyond today's electronics due to their intrinsic quantum nature. The concept of single molecule optoelectronics, which consists in combining optical and electronic properties within a single molecule, strongly emerges in this context. In molecular optoelectronics it is envisioned that light could be used to convey information at high frequency between well-separated components (atoms) within a single-molecule. This objective to access the molecular internal structure and its dynamics is closer thanks to the achievement by researchers at IPCMS of Strasbourg. These researchers implemented a nanoscopic technique which allowed to distinguish the exact origin of a molecular flash inside a molecule at the atomic scale. The team of researchers observed an unexpected blinking of the emitted light from the molecule, and together with theoretician colleagues from the "Theory of Nanophotonics" group at CFM in San Sebastian, they identified and associated the molecule's flash fluctuation to the switching of hydrogen atoms between two positions of the molecule (about 1000 times per second), in a mechanism known as tautomerization. This result provides new information on this reaction, and shows that a molecule may be used as an intermittent emitter, potentially controllable, and relevant for optical communications at the nanoscale.

"Hyper-resolved map of single-molecule light emission achieved"

The researchers used the sharp metallic tip of a scanning tunneling microscope as an optical nanoantenna capable, simultaneously, of confining light to sub-molecular volumes and to excite a single-molecule with electrons. Located on top of a free-base phthalocyanine, a prototypical single-molecule switch, this nanoantenna was capable of amplifying the intensity of the molecular flashes by several orders of magnitude. By scanning the antenna with respect to the molecule, a spatial map of the flash emission was obtained with unprecedented atomic resolution. These results turn the dream of molecular optoelectronics into a closer reality.

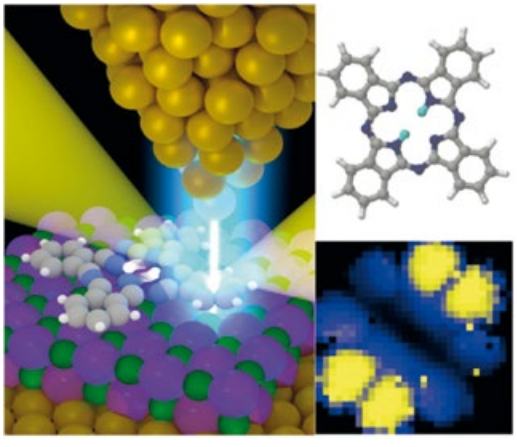


Figure: *(Left) Artistic view of the amplified fluorescence of a molecule induced by a nanoantenna tip. The two central hydrogen atoms are switching positions, and producing specific light flashes. (Right) Top: Structure of the phthalocyanine molecule under study. Bottom: Light-emission map with intramolecular resolution, allowing for identification of the origin of the flashes within the molecule.*

14

Strongly coupled exciton–plasmon nanohybrids reveal extraordinary resistance to harsh environmental stressors: temperature, pH and irradiation

Hendel T, Krivenkov V, Sanchez-Iglesias A, Grzelczak M, and Rakovich YP.

Nanoscale 12, 16875 (2020)

The enhancement of light–matter interaction through strong coupling is a convenient strategy for the development of photonic devices. Usually, the systems under strong coupling regime suffer from poor structural stability. The present study demonstrates outstanding resistance of these structures to harsh stressors.

Hybridized plexcitonic states have unique properties that have been widely studied in many research fields targeted at both fundamental science and innovative applications. However, to make these applications come true, one needs to ensure the stabilization and preservation of electronic transitions in hybrid nanostructures under the influence of external stressors in regimes that have not yet been comprehensively investigated.

Among other strongly coupled structures, localized plasmon/exciton complexes attract special attention because of the possibility to enormously minimize the mode volume in these systems. However, the use of plasmonic nanoparticles as nanoresonators and J-aggregates as quantum emitters imposes specific requirements on the hybrid system, one of which is the stability of exciton–plasmon hybridization under environmental stress.

The present work shows that nanohybrid systems, composed of plasmonic nanoparticles and J-aggregates of organic molecules, display outstanding resistance to harsh environmental stressors such as temperature, pH and strong light irradiation as well as demonstrate long-term stability and processability of the nanostructures both in weak and strong coupling regimes.

Specifically, the spectral features associated both with weak and strong coupling effects in hybrids based on Au nanoparticles and J-aggregates of cyanine dye were found to be stable over several weeks, upon temperature changes between 10 and 70 °C and pH in the range

from 4 to 10. They are also able to withstand high-power irradiation on an unprecedented timescale. In addition, a morphologically induced alteration of the plasmon–exciton coupling strength has been revealed, which is the consequence of the difference in quality factors and local field enhancement generated by nanoparticles of two different shapes. Researches envisage that these findings can be exploited for the development of advanced highly stable devices for optoelectronic, bioimaging and sensing applications. These findings also contribute to a deeper understanding of the physicochemical properties of plexcitonic nanoparticles.

"The present work shows that the nanohybrid system, composed of plasmonic nanoparticles and J-aggregates of organic molecules, displays outstanding resistance to harsh environmental stressors"

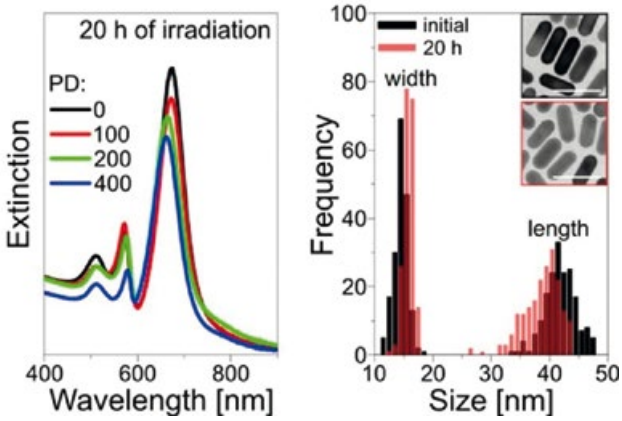


Figure: *Photostability of nanohybrids irradiated with varying power density and size distribution histograms of two hybrid samples (TEM images in inset) before and after irradiation.*

15

Femtosecond laser direct inscription of 3D photonic devices in Er/Yb-doped oxyfluoride nano-glass ceramics

De Aldana JRV, Romero C, Fernandez J, Gorni G, Pascual MJ, Duran A, and Balda R.

Optical Materials Express 10, 2695 (2020)

The present work demonstrates the potential of transparent oxyfluoride nano-glass ceramics co-doped with Er^{3+}/Yb^{3+} ions for the integration of 3D photonic devices by femtosecond laser inscription in the low repetition-rate regime (1 kHz). The results suggest that this target material is an excellent host for the integration of active photonic devices.

The use of ultrashort laser pulses for the inscription of optical waveguides in transparent dielectrics has attracted great attention since the first demonstration due to the intrinsic properties of the technique; the fabrication is direct and can be applied to almost any transparent dielectric, it does not require any specific sample preparation and, more remarkably, it allows the implementation of 3D structures. Among the different substrates used for waveguide inscription by femtosecond laser irradiation, oxifluoride nano-glass ceramics containing rare-earth doped fluoride nanocrystals combine the good mechanical and chemical stabilities of oxide glasses with the low phonon energy of fluoride crystals, thus being of great interest in the operation of active devices.

This collaborative work carried out by the groups led by Javier Vázquez de Aldana (University of Salamanca), Alicia Durán (ICV-CSIC) and Rolindes Balda (CFM, UPV/EHU), demonstrates the potential of transparent oxyfluoride nano-glass ceramics co-doped with Er^{3+}/Yb^{3+} ions for the integration of 3D photonic devices by femtosecond laser inscription. The fabrication is not critical, finding a wide range of irradiation conditions (pulse energy and scanning velocity) in which guiding structures are produced supporting high-quality modes. The technique of multi-scan inscription was successfully applied to tailor the refractive index profile of the waveguides, obtaining multimodal structures. The suitability of the glass-ceramics as substrate for the integration of complex photonic elements was demon-

strated by implementing several splitter designs, both 2D and 3D (Figure 1, left column). The modal profiles at output preserved the single mode behavior at 633 and 800 nm (see normalized intensity for 800 nm in the Figure, central column). The results demonstrate the optimum behavior of Er^{3+}/Yb^{3+} oxyfluoride nano-glass ceramics as a host material for the integration of complex 3D active photonic circuits by femtosecond laser irradiation.

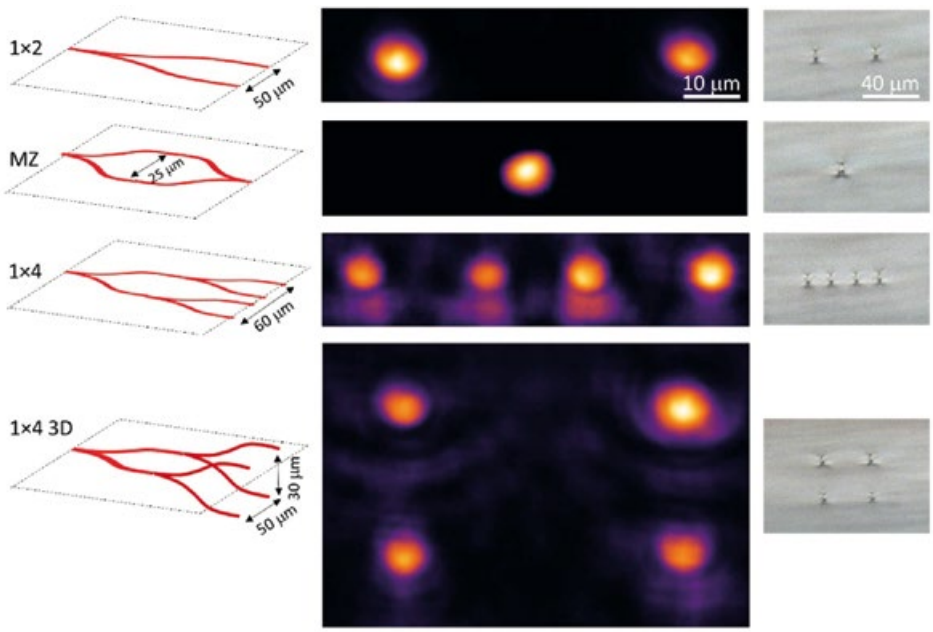


Figure: *Scheme of the implemented photonic elements (left column), normalized near-field modal profiles at 800 nm (central column), and microscopic pictures of the output facet (right column). From top to bottom, 1×2 splitter, Mach-Zehnder interferometer, 1×4 splitter (2D), and 1×4 splitter (3D).*

16

Kerker conditions upon lossless, absorption, and optical gain regimes

Olmos-Trigo J, Sanz-Fernandez C, Abujetas DR, Lasa-Alonso J, de Sousa N, Garcia-Etxarri A, Sanchez-Gil JA, Molina-Terriza G, and Saenz JJ.

Physical Review Letters 125, 073205 (2020)

A nanoantenna with balanced electric and magnetic dipole moments exhibits a directive radiation pattern with zero backscattering. This is known as the first Kerker condition after Kerker, Wang, and Giles, who predicted in 1983 that, under plane wave illumination, magnetic spheres with equal relative permittivity and permeability radiate no light in the backscattering direction. They also concluded that, for certain permittivity and permeability relations for nanospheres, this zero optical light scattering condition happened in the forward direction.

Three decades later, a renewed version of these ideas was proposed for subwavelength dielectric spheres of high refractive index (HRI) materials, reinvigorating the interest on these light scattering conditions. Interestingly, the scattering properties of HRI nanospheres can be fully described by dipolar modes. At the first Kerker condition the electric and magnetic dipolar modes oscillate in phase with equal amplitude. This optical response drives to destructive interference between the scattered fields at the backscattering direction, which is commonly referred to as the zero optical backscattering condition.

This anomalous light scattering condition was first experimentally measured in the limit of small particle in the microwave regime for ceramic spheres and, soon after, in the visible spectral range for HRI Si and GaAs nanospheres.

However, recent results suggest that the concept of small particle is sufficient, but not necessary, to guarantee a dipolar response in the optical scattering of an object. Consequently, the mentioned backscattering anomalies could also be measured on larger dielectric particles.

The absence of backscattered light emerges at the first Kerker condition for dipolar particles regardless of the incoming polarization. On the other hand, for cylindrically symmetric particles, the absence of backscattered light follows from the preservation of electromagnetic helicity. Conservation of helicity has proven crucial in many applications such as enhanced chiral light-matter interactions, or in the spin-orbit interactions of light. Remarkably, it has been reported that from a relatively simple far-field measurement of the electromagnetic helicity at a right angle, the radiation pattern of the dipolar particle is inferable.

Now, a team of researchers analytically demonstrates that either losses or optical gain inhibit the first Kerker condition for homogeneous spheres regardless of the particle's size, incident wavelength, incoming polarization, and multipole order. It follows that dissipating spheres such as dielectric Mie spheres in the visible spectral range and plasmonic particles, such as metal spheres, cannot exhibit the first Kerker condition.

For a germanium (Ge) sphere in the dipolar regime, the team quantifies the gradual drift from the ideal zero optical backscattering condition as the absorption rate is increased. Finally, that optical gain is mandatory to reach the zero forward light scattering condition is demonstrated.

The researchers show that the electromagnetic helicity cannot be preserved after scattering by an arbitrary dielectric sphere in the presence of losses or optical gain. Hence, neither can the zero optical backscattering condition be fulfilled in that scenario.

These results unveil a hidden connection between two symmetries from fundamental principles: energy conservation, mathematically expressed in terms of the optical theorem, and the electromagnetic duality, which is restored at the first Kerker condition. This intriguing link opens new insights into Mie theory.

"This work shows that that either losses or optical gain inhibit the emergence of this condition for homogeneous spheres regardless of the particle's size, incident wavelength, incoming polarization, and multipole order."

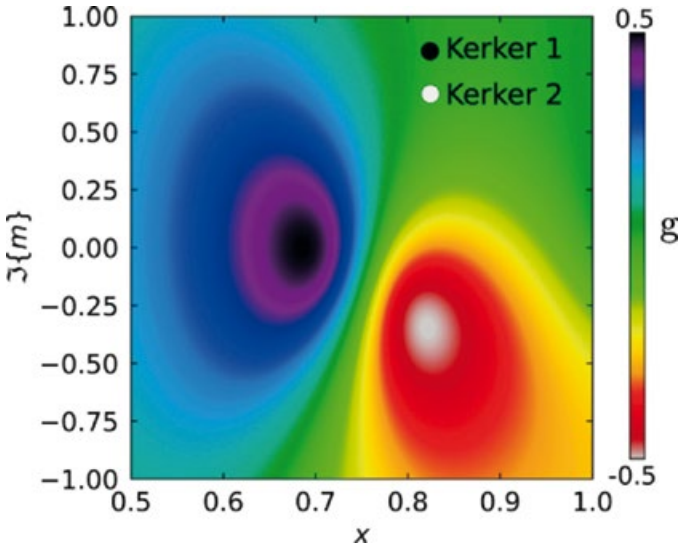


Figure: *(a) Real (dash-dotted red) and imaginary part (dashed-red) of the refractive index contrast (m) vs the incident wavelength (λ) for a Ge sphere. Maximum of the expected value of the EM helicity in solid blue, ⟨Λ⟩max, for a Ge sphere vs λ under plane wave illumination with σ=+1. (b) Color map of ⟨Λ⟩ vs λ and particle's size (R) for a Ge sphere under plane wave illumination with σ=+1. The visible range is encompassed by a dashed rectangle. As mentioned in the text, in this region helicity conservation is never fulfilled.*

17

Coherent structural relaxation of water from meso- to inter-molecular scales measured using neutron spectroscopy with polarization analysis

Arbe A, Nilsen GJ, Stewart JR, Alvarez F, Sakai VG, and Colmenero J.

Physical Review Research 2, 022015 (2020)

Applying recently implemented neutron scattering polarization analysis capabilities at the time-of-flight spectrometer LET (ISIS Neutron and Muon Source, UK), the authors report the separate measurement of the coherent and incoherent dynamic structure factor of heavy water with high resolution and in a wide range of scattering vector for the first time.

The collective dynamics of water in the terahertz range has been intensively investigated since the 1970's. Most studies used Inelastic X-ray Scattering (IXS), and invoked a viscoelastic model that assumes the existence of a "structural" relaxation process. A direct observation by IXS of this relaxation is, however, difficult due to the current resolution of IXS. IXS is also usually limited to mesoscopic scales (scattering vector $0.2 \leq Q \leq 0.7 Å^{-1}$). Thus, the crossover towards the inter-molecular scale ($Q \approx 2 Å^{-1}$ for water) had not been well explored up to now.

Quasielasic Neutron Scattering is the ideal technique to directly observe the structural relaxation in a wide Q-range and with high-energy resolution. However, the intensity always contains coherent and incoherent contributions. The LET spectrometer with polarization analysis allowed separately measuring coherent and incoherent dynamic structure factor of heavy water with sub-meV resolution in a wide Q range (Figure 1). This breakthrough experiment revealed a striking decoupling of collective and single-particle motions completely hidden in previous experiments. At mesoscales, the decorrelation of the collective fluctuations hardly depends on Q. The directly deduced characteristic time for the structural relaxation there agrees well with that deduced from IXS. In the crossover range towards inter-molecular scales, the results are nicely described by

the convolution of a Q-independent mode and diffusion. The combination with Molecular Dynamics simulations carried out at the Materials Physics Centre was very helpful for the data interpretation.

This work is a reference for future studies involving water under different conditions or as one of the components, influencing fields as broad and diverse as biology, soft matter or geology. In addition, it illuminates one of the most crucial open questions for liquids and glass-forming systems: the collective dynamics in the region of intermediate length scales, and how it develops toward the intermolecular ones.

"This work opens a new way of approaching the unknown territory of coherent scattering not only in water under different conditions, but also in H-bonded liquids and glass-forming systems."

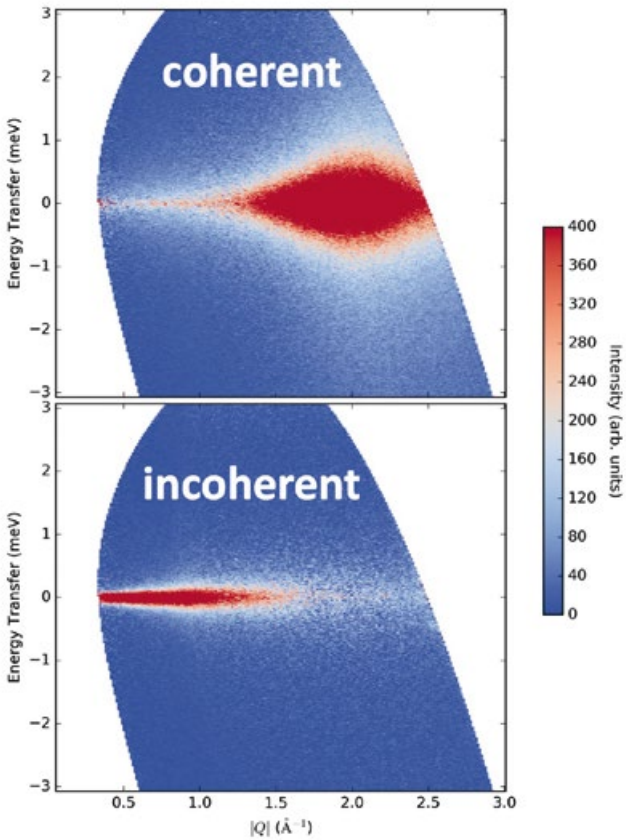


Figure: *Projections of coherent and incoherent contributions to the neutron intensity scattered by D_2O at 295 K and separated by PA.*

18

Direct observation of desorption of a melt of long polymer chains

Monnier X, Napolitano S, and Cangialosi D.

Nature Communications 7, 2292 (2020)

A polymer in contact with an inorganic substrate spontaneously forms bonds via Van der Waals forces at the substrate's surface. Though each of these bonds is intrinsically weak, the presence of numerous pinpoints for each polymer chain results in strong polymer adhesion. This phenomenon, known as polymer adsorption, takes place spontaneously and with reasonably fast kinetics in the polymer melt, underlying the phase transformation from the "standard" unadsorbed to the adsorbed polymer melt, thermodynamically driven by a decrease in the free energy.

The concomitant decrease of enthalpy and entropy in adsorption is analogous to the well-known phenomenon of crystallization. Within this analogy, increasing the temperature entails the progressive enhancement of the entropic part of the free energy and, thereby, the opposite phenomenon – that is, desorption, analogous to melting, is expected on heating [see panel (a) of the Figure]. Unveiling the existence of this scenario by heating has so far remained elusive due to polymer degradation on heating at low rates [dotted line, panel (b) of the Figure]. To circumvent degradation, this study exploits the capabilities of fast scanning calorimetry allowing heat exchange by a material while the temperature is rapidly varied. With this technique, polymer molecules can be brought to high temperature within a fraction of a second, thus preventing degradation [dashed line, panel (b) of the Figure].

Heating scans at 10^4 K/s on poly(t-butyl styrene) (PTBS) samples adsorbed for different times above the glass transition temperature are shown in panel (c) of the Figure. The signature of polymer desorption is an endothermic overshoot at about 660 K, underlying the previous adsorption phenomenon. The position of this overshoot is independent of annealing conditions, highlighting the thermodynamic nature of the transition. The magnitude of the overshoot increases with annealing time, signifying increasing amounts of adsorbed polymer. The time evolution of the enthalpy of desorption at different annealing temperatures is shown in panel (d) of the Figure. Decreasing the adsorption temperature renders adsorption slower. Analysis of temperature dependence of the adsorption time [inset of panel (d) of the Figure] indicates that adsorption is triggered by the same process responsible for the glass transition, that is, the primary relaxation of the polymer.

In summary, fast calorimetry permitted to fully characterize the previously elusive phase transition reverting adsorbed polymer chains to standard desorbed polymer melts. This is an important advance on the state of the art of polymer physics. In addition to such advance of the study of phase transitions, this study paves the way to developing new methods that allows tailoring properties of nanomaterials in applications such as smart coatings, flexible electronics and more. The properties of these innovative systems, in fact, depend on

"Fast scanning rates allows detecting the first order phase transition from adsorbed to desorbed chains, thus allowing tuning the amount of polymer adsorbed on a solid surface"

how many molecules are adsorbed, and, in this work, Monnier et al. anticipate that by adequately mastering the adsorption/desorption transition it is possible to fabricate better performing and more durable materials.

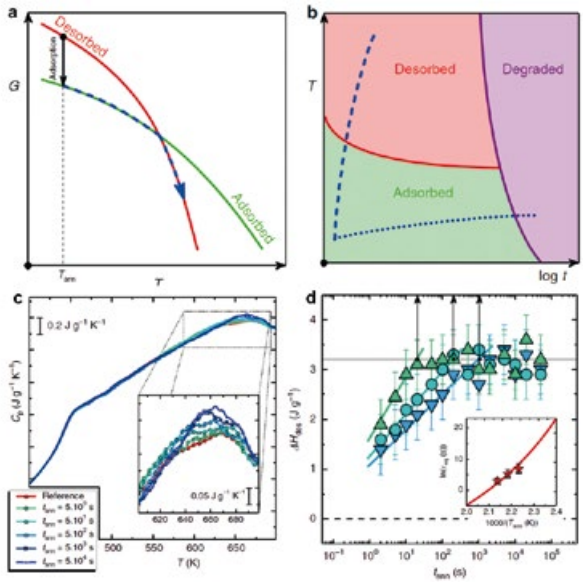


Figure: *(a) Free energy vs. temperature for the desorbed (red line) and the adsorbed (green line) phases. (b) Schematic representation of time–temperature–transformation diagram for an adsorbed polymer layer. The blue dashed line and the dark blue dotted line indicate constant heat transformation at, respectively, fast and slow rate. (c) Heating scans at 10^4 K/s after annealing at 458 K for various times. Inset: enlargement in the temperature range where desorption takes place. (d) Heat of desorption as a function of annealing time, at 448 K (blue), 458 K (cyan) and 468 K (green). Vertical arrows indicate the timescale to reach a plateau in the enthalpy of desorption. Inset: equilibration time as a function of the inverse temperature (stars). The red line depicts the temperature dependence of the relaxation time.*

19

Single-chain nanoparticles: opportunities provided by internal and external confinement

Verde-Sesto E, Arbe A, Moreno AJ, Cangialosi D, Alegria A, Colmenero J, and Pomposo JA.

Materials Horizons 7, 2292 (2020) - REVIEW

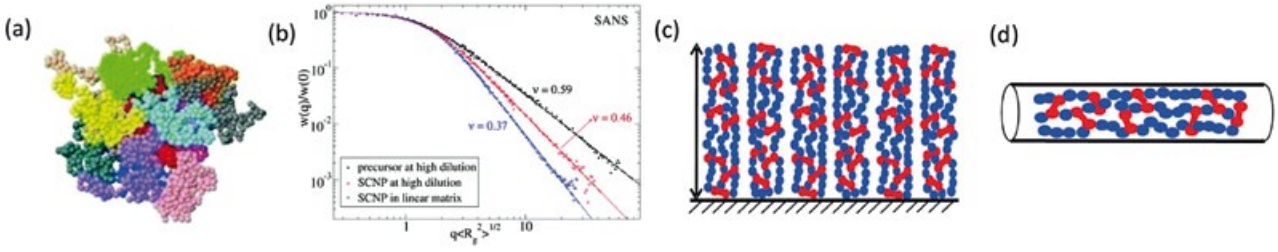
Single-Chain NanoParticles (SCNPs) result from the folding individual synthetic polymer chains by means of multiple intra-chain (reversible or irreversible) bonding interactions. The size of these soft nano-objects can be easily tuned between 3 and 30 nm. Only a rough analogy exists between the process of SCNP formation and the precise, specific folding of a polypeptide chain to its native, functional state (e.g., enzymes). Most SCNPs result in a typical morphology in solution more akin to those displayed Intrinsically Disordered Proteins (IDPs).

Strategies to induce globule formation in SCNPs were also investigated, most of them based on tuning the hydrophobic/hydrophilic balance of the SCNP precursor. The conformational degrees of freedom in SCNPs are severely restricted, giving rise to notorious local domain formation and, hence, to interesting topological self-confinement effects.

Self-confinement in SCNPs has already been exploited for catalysis, encapsulation, transport and delivery of therapeutic cargos, sensing, targeting and bioimaging applications, as well as a variety of other advanced applications. Further progress is expected in these fields accompanied by the development of new methods of rigorous sequence control and precise placement of single functional monomer units at multiple positions along the polymer backbone. This development will presumably lead to precise control of the SCNP topology and, hence, to highly accurate structure–property relationships.

External confinement – as imposed under different geometrical constraints as well as in crowded solutions, in the melt state and on surfaces – is an extra parameter to tune the size, shape, dynamics and, hence, potential functionality/foreseen applications of SCNPs. The unifying vision that results by combining recent experiments, simulations and theory suggests that, in addition to the global size and shape, external confinement also affects the local internal structure of SCNPs and their dynamics, which are critical e.g. for catalysis and drug delivery applications. This recent knowledge opens up new avenues to tune the properties and functionality of SCNPs (see Figure).

"Both self-confinement and external confinement offer a plethora of opportunities to tune the properties of SCNPs for a variety of practical applications"



Hence, innovative purification techniques of SCNPs can be envisioned based on their expected behavior during ultrafiltration through nanopores under an elongational flow field. The compact crumpled globule conformation that sparse SCNPs, adopted under crowding in the melt and in all-polymer nanocomposites, often induces significant viscosity reduction effects that could be beneficial for the development of improved all-polymer nanocomposites. Smart responsive surfaces could be foreseen based on a dense array of SCNPs attached to a surface loaded with active substances to be delivered through stimuli-mediated rupture of intra-chain cross-links. Moreover, new topological nanostructures could result by increasing the complexity of the polymer precursors used for SCNP synthesis, their hydrophobic/hydrophilic balance, self-assembly properties, and so on.

Figure: *Illustration of external confinement imposed on SCNPs: (a) Crumpled globule morphology of sparse SCNPs (drawn in different colours) in a concentrated solution as revealed by MD simulations. (b) Change in conformation of SCNPs on passing from dilute solution (sparse open conformation, scaling exponent ν = 0.46) to all-polymer nanocomposites (crumpled globule conformation, scaling exponent ν = 0.37) as determined by SANS experiments. (c) Schematic illustration of arrays of SCNPs on surfaces. (d) Change in conformation of SCNPs in nanopores.*

20

The instrument suite of the European Spallation Source (ESS)

ESS Collaboration, including Fernandez-Alonso F.

Nuclear Instruments and Methods in Physics Research A 957, 163402 (2020)

The use of the neutron as an exquisite probe of the structure and dynamics of condensed matter is not only well established, but it also continues to evolve in exciting directions, particularly in our continent. Currently under construction in Lund (Sweden), the European Spallation Source (ESS) seeks to offer order-of-magnitude gains in scientific capabilities relative to the state-of-the-art.

The instrument suite described in this work represents the culmination of continued efforts across a wide range of disciplines and institutions over the past decade. The ESS is an accelerator-based, pulsed-neutron source optimized to provide high flux, flexible resolution, and broad bandwidth, capabilities that translate into a plethora of new scientific opportunities. A total of fifteen instruments have been designed to this end, with a view to their imminent construction and subsequent deployment: two small-angle scattering instruments and two reflectometers; an imaging station; five diffractometers for the study of single crystals, macromolecular systems, magnetism, and engineering; and five inelastic neutron spectrometers spanning a wide range of length- and time scales simultaneously – one of the primary merits and strengths of neutron-scattering techniques, as illustrated in the accompanying figure. The team at the Materials Physics Center has been particularly focused on the VESPA spectrometer, including its science case and specification. This task has benefitted greatly from recent and joint developments at other neutron sources worldwide, most notably on TOSCA at the ISIS Pulsed Neutron & Muon Source in the United Kingdom. Both VESPA and TOSCA are high-resolution broadband spectrometers ideally suited to explore the properties of new materials, from fuel stores and nanostructured media to supramolecular frameworks for carbon-dioxide capture. On VESPA, the variable spectral resolution coupled to simultaneous diffraction also paves the way for parametric and kinetic studies that would offer an unprecedented level of detail and insight currently beyond our reach.

"An international team from forty-one institutions across twelve countries introduce the initial instrument suite of the European Spallation Source, currently under construction in Sweden."

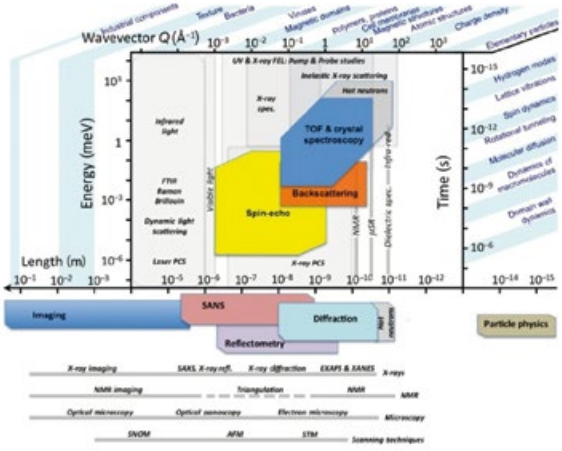


Figure: *Length and time scales accessible to neutrons, along with a qualitative comparison with other experimental probes. Adapted from Fernandez-Alonso F and Price DL,* Neutron Scattering – Fundamentals *(Academic Press, 2013).*

FACILITIES & EXTERNAL SERVICES

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

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 characterisation techniques: X-Ray Photoemission Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), Low Energy Electron Diffraction (LEED) and Scanning Tunnel Microscope (STM) (with the possibility to use in Atomic Force Microscope (AFM) mode). The chamber has two samples preparation chambers, with the required Molecular Beam Epitaxy (MBE) and sample preparation tools.

SURFACE MAGNETISM LAB

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

ULTRA-LOW TEMPERATURE SCANNING TUNNELING MICROSCOPY LAB

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

ELECTRONIC PROPERTIES AT THE NANOSCALE

CERAMICS 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)

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

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 characterise 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 micro-photoluminescence 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 (ThorsLab)

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 stabilised 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 polarisation 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); an 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), polarisers (from Thorlabs and Standa) and Single Photon Counting Modules (SPCM, APDs SPCM-AQ4C model from Excelitas), for analysing 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 centres in diamond

POLYMERS AND SOFT MATTER

DIELECTRIC SPECTROSCOPY LAB

The "Dielectric Spectroscopy" laboratory provides characterisation 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 Depolarisation Currents (TSDC): Novocontrol

MICROSCOPY LAB

The "Microscopy" laboratory allows materials structural characterisation 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 specialised in synthesis of polymers and soft-matter based materials, with special focus on click chemistry methods. This laboratory can characterise 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 CHARACTERISATION LAB

The "Thermal Characterisation" laboratory hosts the following equipment for material characterisation, 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)

REOLOGICAL CHARACTERISATION LAB

The "Reological Characterisation" 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 analyser (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 characterise 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 characterisation 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 characterisation 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) CENTRE

In addition to the experimental facilities, CFM has a High Performance Computing (HPC) Centre that provides scientific computing capabilities and support across all CFM research lines. The CFM Computing Centre consists of two Data Centers hosting four HPC clusters of different sizes, kinds and purposes, all adding up a total of 240 computing nodes with more than 4800 cores and 24TB or RAM. This provides CFM with a computing time of more than 42 million CPU hours a year, and an aggregated computing power of 110 TFLOPS of Theoretical Peak Performance.

There are currently four CFM HPC clusters:

- *Oberon* cluster (the main, general purpose, CFM HPC cluster), composed of 182 computing nodes with two Xeon processors and a memory range of 24 GB up to 256 GB per node, all of them sharing a high speed-low latency Infiniband connection network and a high performance shared parallel filesystem, giving a total of 2000 cores and 15 TB of memory. This cluster gives service to the whole CFM research community.
- *Nostromo* cluster, targeted to shared memory – single node molecular dynamics calculations. It is composed of 17 AMD Opteron 6300 series computing nodes with 64 cores and 64 GB of RAM each node, giving a total of 1088 cores and about 1.1 TB 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 96 GB of memory in each node, with an Infiniband FDR interconnection network, giving a total of 1120 cores and 2.7 TB of memory.
- *Sama* is a multipurpose cluster designed for high-level ab initio electronic structure calculations and molecular dynamics simulations. It is composed of 13 computing nodes with two Intel Xeon Gold 6240R processors (48 cores), 384 GB of memory, and 1 TB NVMe SSD disk per node, all interconnected through an Infiniband HDR 100 Gb/s network, and giving a total of 624 cores and 4.8TB of memory.

These four HPC clusters service a wide range of computational needs in the CFM, mainly related to ab-initio calculations of advanced materials, a transverse topic within the Centre. Apart from these four clusters, 12 workstations are dedicated to running specific numerical applications, and are also used for data analysis and code development and testing. All these equipments are managed by the CFM Scientific Computing Service that, in addition to administering the aforementioned equipments, also provides scientific and general computing advice to the CFM researchers, and organises scientific computing workshops and tutorials.

EXTERNAL SERVICES

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

DIFFERENTIAL THERMAL ANALYSIS (DTA)

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

ISOBARIC THERMAL EXPANSION

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

ABSORPTION SPECTROSCOPY IN TERAHERTZ (THZ) DOMAIN

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

DIELECTRIC CHARACTERISATION

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

MATERIALS SURFACE CHARACTERISATION

The service offers the surface characterisation of materials by means of X-ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoemission Spectroscopy (UPS), Atomic Force Microscopy (AFM) and Scanning Tunnel 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 semiclassical models, molecular dynamics, Monte-Carlo, etc.)

RESEARCH OUTPUT

Among all the articles published at CFM, **81 %** 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
217

Q1 Publications
142

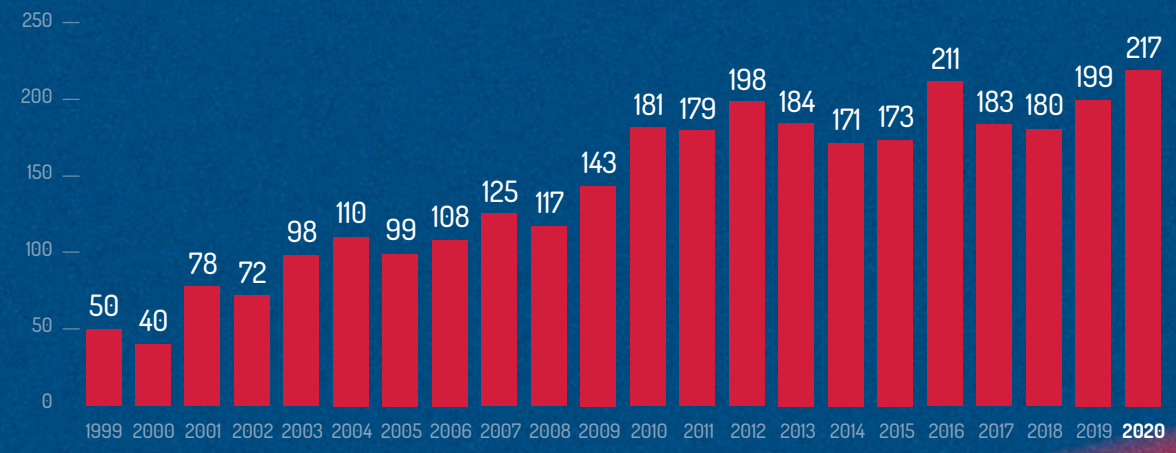
D1 Publications
89

H-Index
133

ISI Web of Science citations
13 021* in 2020

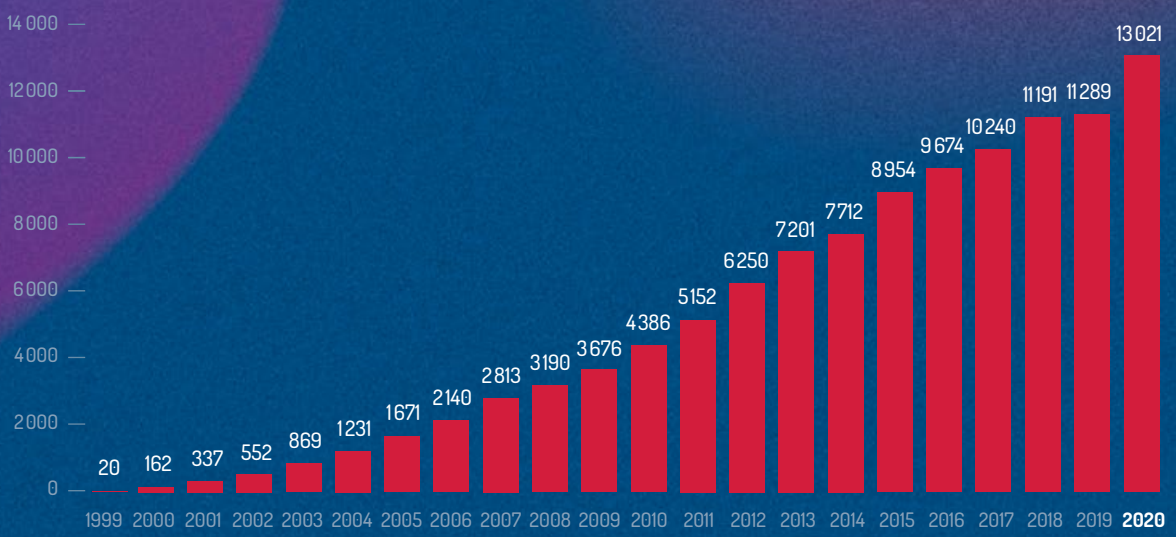
*As of April 2021

PUBLICATIONS



Total number of ISI publications *
since 1999 as of April 2021: **3116**

CITATIONS



Total number of ISI citations since 1999: **117 718**
H index as of April 2021: **133**

Total number of publications with impact factor larger or equal than that of Physical Review Letters:

Journal	Number of articles	Impact factor
Nature	2	42.78
Nature Materials	2	38.66
Nature Nanotechnology	3	31.54
Nature Photonics	1	31.24
Advanced Materials	2	27.40
Nature Physics	1	19.26
Wiley Interdisciplinary Reviews-Computational Molecular Science	1	16.78
National Science Review	1	16.69
Annual Review of Condensed Matter Physics	1	14.83
Journal of the American Chemical Society	3	14.61
ACS Nano	7	14.59
Science Advances	2	13.12
Angewandte Chemie - International Edition	5	12.96
Physical Review X	2	12.58
ACS Catalysis	1	12.35
Materials Horizons	1	12.32
Nature Communications	7	12.12
Nano Letters	7	11.24
Chemical Engineering Journal	2	10.65
Chemical Science	1	9.35
NPJ Computational Materials	1	9.34
2D Materials	1	9.32
ACS Applied Materials & Interfaces	1	8.76
Physical Review Letters	7	8.38

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5 **Resolving segmental polymer dynamics in nanocomposites by incoherent neutron spin-echo spectroscopy**
Musino D, Oberdisse J, Farago B, Alegria A, and Genix AC.
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6 **Cyclic polyethylene glycol as nanoparticle surface ligand**
Aboudzadeh MA, Iturrospe A, Arbe A, Grzelczak M, and Barroso-Bujans F.
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7 **Present and future of surface-enhanced Raman scattering**
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8 **Band depopulation of graphene nanoribbons induced by chemical gating with amino groups**
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12 **Multiscale analysis of phase transformations in self-assembled layers of 4,4 '-Biphenyl dicarboxylic acid on the Ag(001) Surface**
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Kimera (Software)

Authors: Pablo Martín, Hegoi Manzano Moro, and Jorge Sánchez Dolado.

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Method for colorimetric detection of bacteria in food samples

Authors: María Jesús Grilló Dolset, Victoria Eugenia Garrido González, Javier Aizpurua Iriazabal, María Sanromán Iglesias, Marek Grzelczak, and Inés Echeverria Goñi.

20382599

Sensible thermal energy storage media based on alkali activated concrete

Authors: Jorge Sánchez Dolado, Guido Goracci, Pavel Martauz, and Cvopa Branislav.

20157518

Superconducting electromagnetic wave sensor

Author: F. Sebastian Bergeret Sbarbaro, Francesco Giazotto, Tero Heikkila, and Ilari Maasilta.

WO 2019/058357 Al

Superconducting logic element

Authors: Francesco Giazotto, Elia Strambini, Giorgio De Simoni, and F. Sebastian Bergeret Sbarbaro.

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BOOK CHAPTERS

Dynamics of water in partially crystallized solutions of glass forming materials and polymers: Implications on the behaviour of bulk water

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Magnetic impurities on surfaces: Kondo and inelastic scattering

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Natural topological insulator heterostructures

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TRAINING ACTIVITIES

As a joint center which belongs to the University of the Basque Country (UPV/EHU), the training activity at CFM includes the participation in both the Master and PhD program through the Department of Material Physics of UPV/EHU, as well as setting complementary training activities, 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.

It should be noted that, despite the health emergency in 2020, the tremendous effort made by the UPV/EHU and its teaching staff made it possible to adapt the teaching format and continue teaching at all levels, including the Undergraduate and Master's degree classes in which many of our researchers typically participate.

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. CFM encourages the research groups to hire post-doctoral researchers through internal calls, which support around 2-3 post-doc positions every year. Each research group makes an individual follow-up and training of these young researchers.

PHD PROGRAM: PHYSICS OF NANOSTRUCTURES AND ADVANCED MATERIALS

"Physics of Nanostructures and Advanced Materials" is a PhD program of UPV/EHU that has been recognized as a highly qualified PhD program by the Spanish Ministry of Education (MEE2011-0591 citation of excellence). Within this program, 62 PhD students develop their research fully embedded in the daily life of the research groups in the center.

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

DEFENDED PHD THESES

- **Computational investigations of single-chain nanoparticles: Novel synthesis routes, complex flow behavior and reversible gel formation**
  Author: Maud Formanek
  Supervisor: Ángel Moreno Segurado
  Group: Polymers and Soft Matter
  19/01/2020

- **Quantum transport in nanowires with spin-orbit interaction effect of quasi-bound states**
  Author: Alba Pascual Gil
  Supervisors: F. Sebastián Bergeret Sbarbaro and Vitaly Golovach
  Group: Mesoscopic Physics
  03/03/2020

- **Molecular assembly and reactions on surfaces characterized by low-temperature canning probe techniques**
  Author: Ana Barragán Durán
  Supervisor: Lucia Vitali
  Group: Spectroscopy at the Atomic Scale
  20/03/2020

- **Numerical simulations for the nonequilibrium control of quantum materials**
  Author: Gabriel Topp
  Supervisors: Michael Sentef and Ángel Rubio Secades
  Group: Nano-Bio Spectroscopy
  22/04/2020

- **Novel approaches in quantum chemistry: Self-consistent density-functional embedding and polaritonic coupled-cluster theory**
  Author: Uliana Mordovina
  Supervisors: Daniela Pfannkuche and and Ángel Rubio Secades
  Group: Nano-Bio Spectroscopy
  27/04/2020

- **On the interface of quantum electrodynamics and electronic structure theory: Cavity QED**
  Author: Christian Schaefer
  Supervisors: Michael Ruggenthaler and Ángel Rubio Secades
  Group: Nano-Bio Spectroscopy
  13/05/2020

- **Mixed quantum-classical dynamics in cavity quantum electrodynamics**
  Author: Norah Hoffmann
  Supervisors: Neepa Maitra and Ángel Rubio Secades
  Group: Nano-Bio Spectroscopy
  02/06/2020

- **An efficient Ab-Initio non-equilibrium Green´s function approach to carriers dynamics in many-body interacting systems**
  Author: Fabio Covito
  Supervisors: Daniela Pfannkuche and Ángel Rubio Secades
  Group: Nano-Bio Spectroscopy
  13/07/2020

- **Synthesis and characterization of cyclic polyethers with controlled orientation of the dipolar moment along the chain contour**
  Author: Jordan Ochs
  Supervisor: Fabienne Barroso Bujans
  Group: Polymers and Soft Matter
  09/09/2020

- **Anharmonic effects in thermoelectric and 2D materials**
  Author: Unai Aseguinolaza Aguirreche
  Supervisors: Ion Errea Lope and Aitor Bergara Jauregi
  Group: Quantum Theory of Materials
  18/09/2020

- **Spin-and valley-dependent transport in hybrid system and 2D Dirac materials**
  Author: Xianpeng Zhang
  Supervisors: F. Sebastián Bergeret Sbarbaro and Miguel Ángel Cazalilla Gutiérrez
  Group: Mesoscopic Physics
  12/12/2020

- **Many electrons and the photon field: The many-body structure of nonrelativistic quantum electrodynamics**
  Author: Florian Konrad Friedrich Buchholz
  Supervisors: Michael Ruggenthaler and Ángel Rubio Secades
  Group: Nano-Bio Spectroscopy
  24/11/2020

SHORT STAYS IN FOREIGN UNIVERSITIES

A very important aspect of the PhD training program consists of supporting short stays in foreign universities and centers for PhD students. This year 6 PhD students have 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 2020:

- **José Reina Gálvez**
  Universidad Nacional de San Martín, Buenos Aires (Argentina)
  29 February – 31 May

- **Masoud Mansouri**
  Boston University (USA)
  19 February - 8 May

- **Alvaro Nodar Villa**
  Macquarie University, Sidney (Australia)
  3 March - 10 May

- **Fernando García Martinez**
  Lund University (Sweden)
  4 October - 8 December

- **Mariarita Paciolla**
  University of Viena (Austria)
  9 September - 10 December

- **Cristina Mier González**
  IPCMS Strasbourg (France)
  21 September - 13 December

MASTER EDUCATION PROGRAM

MASTER IN NANOSCIENCE

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

In addition, during their Master's thesis work, the students choose to develop the skills either in fields directly linked with applied and technology-oriented research work in technological centers, or in the basic/oriented research that is carried out in academic research groups. The students will also be able to start developing the research work that may allow them to access the PhD program.

Once again, we must thank the extra effort made by professors and students to ensure compliance with the strict security measures required by the situation, and emphasise that this has not been detrimental to the number or quality of the Master theses defended in 2020.

SCHOLARSHIPS

The Materials Physics Center (MPC) association, together with the Donostia International Physics Center (DIPC), offers scholarships to highly motivated graduates who are planning to complete their studies with a Master's degree.

Furthermore, the MPC and DIPC collaborate with the Gipuzkoa Coopera project and Women for Africa foundation in the framework of the "Learn Africa" program with the aim of facilitating the professional growth of young African women scientists offering a grant that fully covers the stay and expenses of a student to enroll in the Master in Nanoscience program.

In 2020, five graduates were awarded scholarships for the Master in Nanoscience program:

- **Andrés Felipe Bejarano**
  Supervisor: Thomas Frederiksen (DIPC)
- **Harriet Kumi**
  Supervisor: Gabriel Molina Terriza (CFM)
- **Jean Pierre Inchaustegui Revoredo**
  Supervisors: Ángel Alegría Loinaz (CFM) and Daniel Martínez Tong (CFM)
- **Josu Diego López**
  Supervisor: Ion Errea Lope (CFM)
- **Nathaniel Andrés Capote Robayna**
  Supervisors: Alexey Nikitin (DIPC) and Pablo Alonso González (University of Oviedo)

THESES OF THE NANOSCIENCE MASTER SUCCESSFULLY DEFENDED IN 2020

- **Infrared nanoimaging of ultraconfined surface phonon polaritons in MoS2-quartz heterostructures**
  Author: Petr Liska
  Supervisor: Rainer Hillenbrand (CIC nanoGUNE)

- **On the modelling of AFM-based nano-dielectric spectroscopy**
  Author: Jean Pierre Inchaustegui Revoredo
  Supervisors: Ángel Alegría Loinaz (CFM) and Daniel Martínez Tong (CFM)

- **Graphene nanoribbons with Carboxyl edge groups: On-surface synthesis and electronic characterization**
  Author: Lucie Pavlásková
  Supervisors: Aran García-Lekue (DIPC) and Martina Corso (CFM)

- **Anisotropy effect of nanostructure in the mechanical behaviour of pearlitic steel**
  Author: Aritz Dorronsoro Larbide
  Supervisor: Jon Alkorta Barragán (CEIT)

- **Anisotropic phonon polaritons in twisted biaxial Van der Waals crystal slabs**
  Author: Nathaniel Andrés Capote Robayna
  Supervisors: Alexey Nikitin (DIPC) and Pablo Alonso González (University of Oviedo)

- **DNA-Polymer hybrid nanostructures for stimuli-responsive systems**
  Author: Diego Ramírez Revilla
  Supervisor: Thomas Schäfer (UPV/EHU)

- **Strongly coupled plasmon-exciton hybrid nanostructures**
  Author: Emilie Dupont
  Supervisor: Marek Grzelczak (CFM) and Yury Rakovich (CFM)

- **Chemiluminescent single-chain nanoparticles for sensing cobalt ions**
  Author: Andrea Aguirre Baños
  Supervisors: José A. Pomposo Alonso (CFM) and María Ester Verde Sesto (CFM)

- **Endowing single-chain nanoparticles with fluorescent and drug delivery properties**
  Author: Arianne Encinar Manzano
  Supervisors: José A. Pomposo Alonso (CFM) and María Ester Verde Sesto (CFM)

- **Towards the development of novel bicolor sensor for neutrino detection**
  Author: Lander Murillo Lekuona
  Supervisors: Celia Rogero Blanco (CFM)

- **Real-time manipulation of optical trap with deformable mirror**
  Author: Harriet Kumi
  Supervisor: Gabriel Molina Terriza (CFM)

- **Charge-density-wave transition in VSe2 from first principles**
  Author: Josu Diego López
  Supervisor: Ion Errea Lope (CFM)

- **Development of smart substrates for enhancing in near-field spectroscopy**
  Author: Alba Viejo Rodríguez
  Supervisor: Rainer Hillenbrand (CIC nanoGUNE)

- **Electron quantum transport in generic tight-binding models**
  Author: Andrés Felipe Bejarano Sánchez
  Supervisor: Thomas Frederiksen (DIPC)

OTHER MASTER THESES PROJECTS SUPERVISED BY CFM STAFF AND SUCCESSFULLY DEFENDED IN 2020

- **Proximity effects in superconductor-ferromagnetic insulator bilayers of arbitrary thickness**
  Author: Maxime Infuso
  Supervisor: F. Sebastián Bergeret Sbarbaro (CFM)

- **Synthesis of poly(methacrylic-co-polyethylene glycol methacrylate) copolymers and its application on cementitious formulations**
  Author: Sara Pavo Belderrain
  Supervisors: José Ramón Leiza (Polymat, UPV/EHU) and Jorge Sánchez Dolado (CFM)

- **Tailoring the electronic properties of graphene nanoribbons by chemical substitution**
  Author: Iñigo Delgado Enares
  Supervisors: Daniel Sánchez Portal (CFM) and Aran García-Lekue (DIPC)

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.

END OF COURSE PROJECTS AND SHORT STAY VISITS

In the framework of this teaching activity, undergraduate students can join a research group at CFM for a short stay or to fulfill their End of Course Project during the academic year. However, following the health security protocolos in place during 2020, this program was significantly downsized. CFM hosted the visit of two students, Aimar Marauri Iriberri (supervised by Marek Grzelczak) and Eric Gómez Urreizti (supervised by Ángel Alegría) in short stay visits, and one end of course project was fullfiled and defended at CFM premises.

- **Estudio de mezclas poliméricas basadas en polifuranoatos mediante calorimetría diferencial de barrido**
  Author: Julen Olasagasti Imizcoz
  Supervisors: Ángel Alegría Loinaz (CFM) y Daniel E. Martínez-Tong (CFM)
  Group: Polymers and Soft Matter
  End of course project

INTERNSHIPS

CFM also offers the possibility to receive support for this training through different grant programs. In 2020 one person was granted:

- **Julen Olasagasti Imizcoz**
  Supervisor: Silvia Arrese-Igor Irigoyen (CFM)
  Group: Polymers and Soft Matter

WORKSHOPS, CONFERENCES AND SEMINARS

Despite the sanitary emergency, CFM scientists organized or co-organized 9 international workshops and conferences during 2020, out of which 6 had to be finally cancelled. Many of these meetings have been historically 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. Again, this activity was dramatically affected by the COVID19 crisis.

The list of conferences, courses, workshops and seminars organized or co-organized by CFM researchers during 2020 follows:

Total Energy and Force Methods 2020

Organizers: Ivo Souza (CFM), Ion Errea (CFM) and Aran García-Lekue (DIPC).

Carlos Santamaría Centre, UPV/EHU, Donostia / San Sebastián

8-10/01/2020

Software Carpentry Workshop

Instructors: Iñigo Aldazabal, Sonia Olaechea, Ainhoa Oliden, and Tineke van den Berg.

Helpers: Unai Aseguinolaza, Abel Carreras, Meritxell García, Mikel Iraola, Alvaro Nodar, and Xiang Xu.

CFM (CSIC, UPV/EHU, MPC), Donostia / San Sebastián

14, 15, 16 and 23/01/2020

RSC Statistical Mechanics and Thermodynamics Group

Organizers: Carlos Avendaño, Fernando Bresme, Félix Fernández, Manon Higgins-Bos, Susan Little, Andrew Masters, Martin Trusler, Karl Travis, and Patrick Warren.

Online

08/2020 (ongoing series)

PhD SEMINAR SERIES

Since 2013, a regular series of seminars delivered by PhD students is organized at CFM. This activity continued during 2020, mainly, in an online format as webinars. In each seminar, two PhD students present updated results of their respective theses work to the full CFM research community. Two other PhD students assume the role of opponents and are in charge of asking questions and discussing the presented results. The most important goal of this activity is to train PhD students in the necessary habits of science communication and research discussions. Furthermore, it helps to improve the internal communication about the research activity going on in the Center. The list of student seminars given in 2020 follows:

- **Study of the coadsorption of (O, CO) on Ru(0001)**
  Auguste Tetenoire
  22/01/2020

- **Transition-metal oxide chains: spin phases, magnetic anisotropy and coupling**
  Joseba Goikoetxea Perez
  22/01/2020

- **Mean field Hubbard method for non-equilibrium electron transport**
  Sofia Sanz Wuhl
  19/02/2020

- **Kerker conditions in lossless, absorption and optical gain regimes**
  Jorge Olmos Trigo
  19/02/2020

- **Fluorescent single-chain polymer nanoparticles based on Aggregation-Induced Emission (AIE) molecules**
  Julen de la Cuesta Leone
  11/03/2020

- **Synthesis and characterization of cyclic poly(glycidyl phenyl ether) with controlled dipolar microstructure**
  Jordan Ochs
  11/03/2020

- **Symmetry-protection of multiphoton states of light**
  Jon Lasa Alonso
  28/05/2020

- **Isolating Mie resonances in a dielectric sphere using angular momentum beams**
  Martín Molezuelas Ferreras
  28/05/2020

MORE SEMINARS HOSTED BY CFM

- **Taming complex fluids with external fields**
  Fernando Bresme
  07/02/2020

- **Sub-Terahertz Spin Pumping from an Insulating Antiferromagnet**
  Enrique del Barco
  11/02/2020

- **Atomic-scale spin-sensing with a single molecule at the apex of a scanning tunneling microscope**
  Benjamin Verlhac
  20/02/2020

- **The polar surfaces of the delafossite oxides: from massive Rashba spin-splittings to itinerant surface ferromagnetism**
  Federico Mazzola
  09/03/2020

- **Computational Modelling of Metal-Organic Frameworks**
  Rémi Pétuya
  17/09/2020

- **Biological processes at cellular membranes - New knowledge through the use of neutron and X-ray Scattering**
  Marité Cárdenas
  18/11/2020

- **Porous materials at nanoscale - A neutron scattering insight**
  Margarita Russina
  24/11/2020

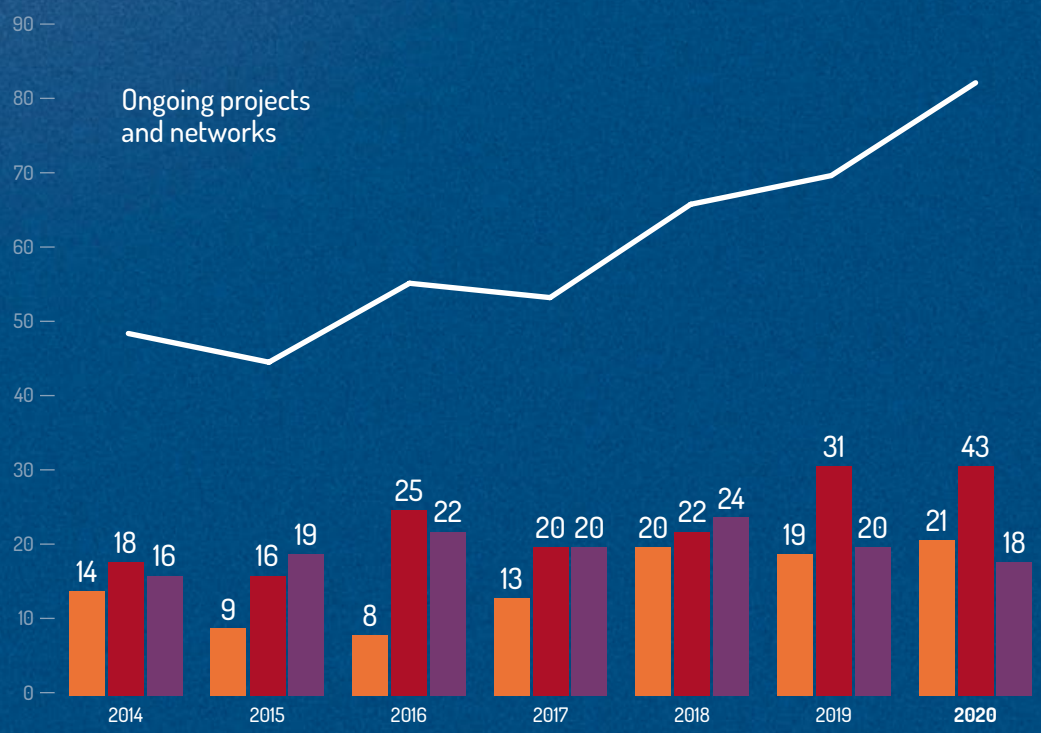
- **Nuclear Quantum effects enter the mainstream**
  Matthew Krzystyniak
  30/11/2020

- **Tailoring the interfacial assembly and the mechanical response of colloidal and biological systems**
  Armando Maestro
  02/12/2020

- **Neutron scattering and complementary investigations of fullerene solutions and polymer nanocomposites thin films**
  Timur Tropin
  04/12/2020

COMPETITIVE FUNDING FOR RESEARCH PROJECTS

RESEARCH PROJECTS AND NETWORKS	Competitive public fundraising in 2020
BASQUE	415 644,34 €
SPANISH	1 522 011,31 €
INTERNATIONAL	1 926 522,85 €
MPC-BERC	1 224 640,00 €
TOTAL	**5 088 818,50 €**



The projects and networks ongoing during 2020 (a total of 82 projects/networks) are listed below according to the source of competitive funding.

BASQUE RESEARCH PROJECTS AND NETWORKS

- **EJ/GV, EKIZIEN 2019: Adquisición Equipamiento Científico, EC19-27**
  Recycling preparative SEC/GPC
  PI: Josetxo Pomposo Alonso

- **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, IKERTALDE 2019, Grupo Consolidado IT1182-19**
  Grupo de Espectroscopía Láser y Materiales Fotónicos
  PI: Rolindes Balda de la Cruz

- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1260-19**
  Desarrollo de nuevas metodologías en problemas destacados de Física de la Materia Condensada
  Partners: Ion Errea Lope; Aitor Bergara Jauregui

- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1255-19**
  Nanophysics 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 Iriazabal
  co-PI: Nerea Zabala Unzalu

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

- **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, Proyectos de Investigación Básica y/o Aplicada 2018-2020 (PIBA), PIBA2018_1_0024**
  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, Proyectos de Investigación Básica y/o Aplicada 2020-2022 (PIBA), PIBA2020_1_0017**
  Hacia la computación cuántica topológica manipulando átomos en superconductores
  PI: Deungjang Choi

- **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, Gipuzkoa Coopera 2020, 2020-IZEN-000012-01**
  ELLAS INVESTIGAN VI: Afrikar emakumezko ikertzaile batek egonaldi bat egin dezan MPCn / ELLAS INVESTIGAN VI: Estancia de investigación en el MPC de una investigadora africana

BASQUE RESEARCH PROJECTS AND NETWORKS

- **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: Josetxo 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

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2020 RED2020, 2020-CIEN-000009-01**
  Estudio de materiales fotovoltaicos de última generación mediante técnicas neutrónicas, microscopía y espectroscopia túnel, y cálculos de primeros principios
  PI: Félix Fernández Alonso

- **Biozientziak Gipuzkoa Fundazioa, Convocatoria de Proyectos de I+D+i COVID-19**
  DETENTE SARS - Detección mediante técnicas físico-químicas específicas y ultrasensibles de SARS-CoV-2
  PI: Celia Rogero Blanco

- **UPV/EHU, Azpiegitura Zientifikoa/Infraestructura Científica 2020, INF 20/03**
  Reómetro rotacional para polímeros y materia blanda
  PI: Juan Colmenero de León

- **UPV/EHU, EHUko Sailentzako Laguntzak/Ayudas Departamentos UPV 2020, DEP20/61**
  Polímeros y materiales avanzados: Física, química y tecnología
  PI: Iñaki Juaristi Oliden

- **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

SPANISH RESEARCH PROJECTS AND NETWORKS

- **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, FIS2016-77188-P**
  Teoría y simulación de fenómenos ópticos y de transporte en materiales girotrópicos
  PI: Ivo Souza

- **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

- **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

- **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, Ikerbasque)

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

SPANISH MINISTRY RESEARCH PROJECTS AND NETWORKS

- **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, Ikerbasque)

- **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, Ikerbasque)

- **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
  Lab Technician: Amaia Iturrospe Ibarra
  Supervisor: Arantxa Arbe Méndez

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

- **Contratos Juan de la Cierva – Incorporación (JdC-I) 2017, IJCI-2017-31600**
  Polymers and Soft Matter: Nanostructures and physical properties at the nanoscale
  PI: Daniel Enrique Martínez Tong
  Supervisor: Ángel Alegría Loinaz

- **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: Deungjang 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: Josetxo Pomposo Alonso

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

- **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, Network Coordinator: Sara Barja Martínez

- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-104650GB-C21**
  Dinámica en soluciones acuosas de polímeros y biopolímeros (subproyecto coordinador)
  Proyecto Coordinado: BRIDGE – Cerrando la brecha entre los polímeros sintéticos y los biopolímeros – propiedades físicas y químicas
  PI: Silvina Cerveny Murcia
  Co-PI: Gustavo A. Schwartz Pomeraniec

- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-107396GB-I00**
  GASOLIN – Interfaces gas/sólido: acoplamiento entre la dinámica nuclear y la dinámica electrónica
  PI: Maite Alducin Ochoa
  Co-PI: Ricardo Díez Muiño

SPANISH MINISTRY RESEARCH PROJECTS AND NETWORKS

- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-105488GB-I00**
  2EDiSNa - Excitaciones electrónicas y dinámicas en superficies y nanoestructuras
  PI: Andrés Ayuela Fernández
  Co-PI: Silkin Vyacheslav (DIPC, Ikerbasque)

- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-107432GB-I00**
  QUATOPHOT - Estudio de los efectos cuánticos en nanofotónica a escala atómica
  PI: Javier Aizpurua Iriazabal
  Co-PI: Rubén Esteban Llorente

- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-103910GB-I00**
  VIMAGSOC - Vibraciones y magnetismo en sistemas nanoscópicos con acoplamiento spin-órbita
  PI: Andrés Arnau Pino
  Co-PI: Asier Eiguren Goyenechea (UPV/EHU)

- **Proyectos de I+D+i de Retos Investigación 2019 (RTI2019), PID2019-111772RB-I00**
  QUATH - Análisis cuantitativo de la contribución de cargas calientes y efecto térmico en fotocatálisis asistida por efecto plasmónico
  PI: Marek Grzelczak
  Co-PI: Jon Mattin Matxain Beraza (UPV/EHU)

- **Proyectos de I+D+i de Retos Investigación 2019 (RTI2019), PID2019-107338RB-C63**
  FunMolSys - Síntesis en Superficie de Sistemas Moleculares Funcionales (subproyecto)
  Proyecto Coordinado: MONOMET - Transferencia de sistemas moleculares funcionales a superficies no metálicas
  PI: Martina Corso
  Co-PI: Dimas García de Oteyza Feldermann (DIPC, Ikerbasque)

- **Proyectos de I+D+i de Retos Investigación 2019 (RTI2019), PID2019-107338RB-C66**
  TheoFunMolSys – Teoría de propiedades electrónicas, topológicas, magnéticas y vibracionales de nanoSistemas Moleculares Funcionales (subproyecto)
  Proyecto Coordinado: MONOMET – Transferencia de sistemas moleculares funcionales a superficies no metálicas
  PI: Daniel Sánchez Portal
  Co-PI: Arantzazu García Lekue (DIPC, Ikerbasque)

- **Contratos Personal Técnico de Apoyo (PTA) 2019, PTA2019-018134-I**
  Apoyo técnico de los laboratorios de ultra-alto vacío del Centro de Física de Materiales (CFM)-Centro Mixto CSIC-UPV/EHU
  Lab Technician: Laura Fernández Gómez-Recuero
  Supervisor: Martina Corso

- **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

- **Acciones de Dinamización Europa Excelencia 2020, EUR2020-112116**
  ARTS – Atomic research for topological superconductors / Investigación atómica para superconductores topológicos
  PI: Deungjang Choi

- **Acciones de Dinamización Europa Excelencia 2020, EUR2020-112066**
  ReversO_2 – Oxygen conversion reactions: Fundamental insights for rational design
  PI: Sara Barja Martínez

- **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)

SPANISH MINISTRY RESEARCH PROJECTS AND NETWORKS

- **CSIC, Programa de Apoyo a la Infraestructura (PAI) 2019-2020, PAI 06-3356**
  Implementación del nuevo laboratorio de síntesis

- **CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2019, 2019AEP061**
  Teoría de nanoestructuras moleculares funcionales para dispositivos optoelectrónicos
  PI: Daniel Sánchez Portal

- **CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2019, 2019AEP062**
  Nanoestructuras moleculares funcionales para dispositivos optoelectrónicos: Guiando reacciones en superficies
  PI: Martina Corso

- **CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2019, 2019AEP042**
  Excitaciones electrónicas en superficies y nanoestructuras
  PI: Andrés Ayuela Fernández

- **CSIC, I-LINK+ 2019, Colaboración Científica Internacional, LINKC20002**
  On-surface polymerization for high performance (opto)electronics
  PI: Martina Corso

- **CSIC, I-COOP+ 2019, Cooperación Científica para el Desarrollo, COOPB20432**
  Diluted magnetic quantum dots assemblies for innovative spintronics
  PI: Martina Corso

- **CSIC, Fondo de Apoyo a los Servicios Científico-Técnicos (FAS) 2020, FAS2020_058**
  Unidad de control para TPS SPECTRA 3000

- **CSIC, Fondo de Apoyo a los Servicios Científico-Técnicos (FAS) 2020, FAS2020_059**
  Sistema de refrigeración para TPS SPECTRA 3000

- **CSIC, Programa de Apoyo a la Infraestructura (PAI) 2020-2021, PAI2020_4026**
  Adecuación de laboratorios de ciencia de superficies del CFM

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

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

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

- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN 01-2016-2017), GA 766864**
  MEMO-Mechanics with Molecules
  PI: Nicolás Lorente Palacios

- **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) V C: Interregional Cooperation, Aquitania-Euskadi-Navarre Euroregion Projects 2017**
  DINaMO-FiVe – Durabilidad de Infraestructuras en ambiente marino: Nano-Materiales Optimizados como Fibras Verdes
  PI: Silvina Cerveny Murcia

- **Setting up European or International Scientific Networks (Montage de Réseaux Scientifiques Européens ou Internationaux, MRSEI) Instrument, ANR-18-MRS1-0014**
  NaWaGui - Nanostructured Waveguides for Photonics
  PI: Rolindes Balda de la Cruz

- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN 01-2016-2017), GA800923**
  SUPERTED - Thermoelectric detector based on superconductor-ferromagnet heterostructures
  PI: Sebastián Bergeret Sbarbaro
  Co-PI: Celia Rogero Blanco

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

- **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 2017, CA17139**
  EUTOPIA - European Topology Interdisciplinary Action
  Management Committee Member: 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 cementitious nanocomposites for heat storage in buildings using Phase Change Materials
  PI: Jorge Sánchez Dolado

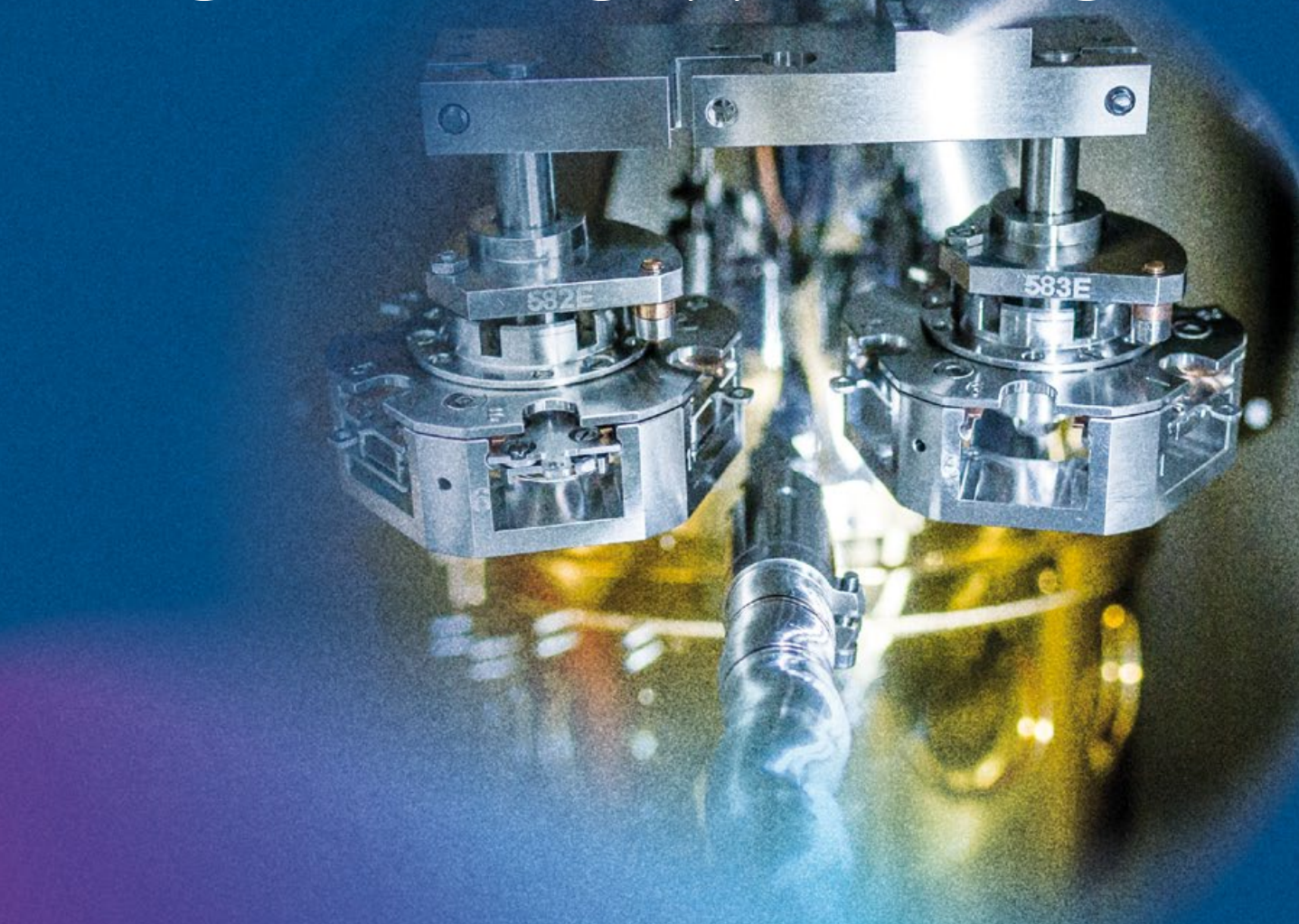
- **Marie Curie Individual Fellowship (H2020-MSCA-IF-2018), GA 839237**
  PhotoWann - Bulk Photovoltaic effect via Wannier functions
  Supervisor: Ivo Souza

- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN-01-2018-2019-2020), GA 861980**
  POSEIDON - NanoPhOtonic devices applying SElf-assembled colloIDs for novel ON-chip light sources
  PI: Javier Aizpurua Iriazabal

- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN-01-2018-2019-2020), GA 863170**
  ArtiBLED - Engineered Artificial Proteins for Biological Light-Emitting Diodes
  PI: Pedro Braña Coto

- **NMBP. Integration of Energy Smart Materials in non-Residential Buildings, LC-EEB-01-2019 (H2020-NMBP-EEB-2019), GA 870114**
  NRG-Storage - integrated porous cementitious Nanocomposites in non-Residential building envelopes for Green active/passive energy STORAGE
  PI: Jorge Sánchez Dolado

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 2020. 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

Kutxa Fundazioa
Scientific cultural activities

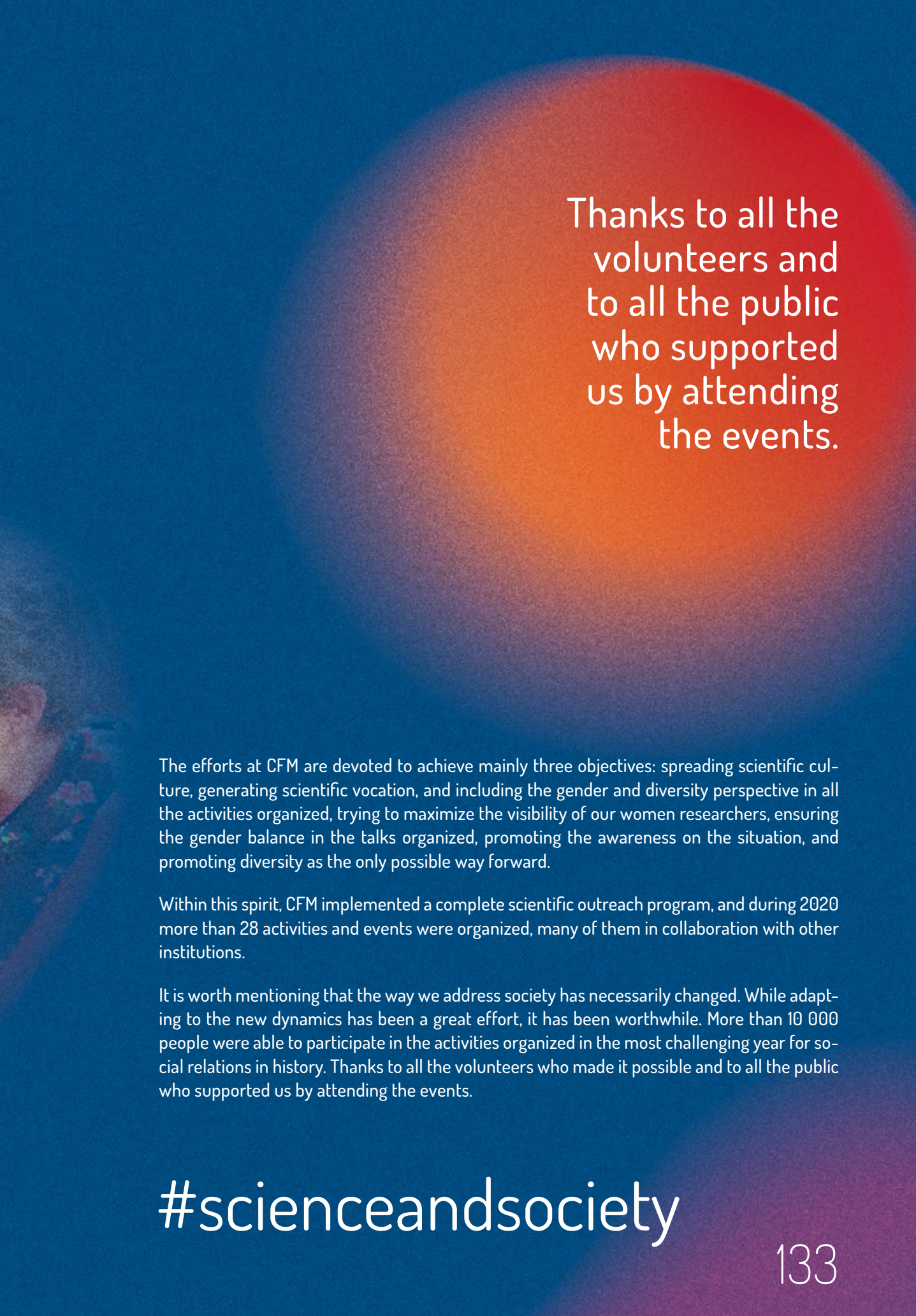
CFM also tackles strong collaborations devoted to technological transfer towards the Basque Industrial Network, within the framework of the ELKARTEK program from the Department of Industry of the Basque Government, as well as towards the European Industrial Network (see Research Funding section).

SCIENCE AND SOCIETY

The pandemic we are living through has brought a crucial issue to the table: the need for the bulk of the public to have the tools to understand the flood of scientific data and information that has come their way. At CFM, supporting scientific culture has been a core policy in our understanding of the scientific community's duty to society.

Developing a so-called "scientific culture" in the public has become crucial these days. 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, pre-doctoral researchers and science communicators.

More than **10 000** people were able to participate in the activities organized in the most challenging year for social relations in history



Thanks to all the volunteers and to all the public who supported us by attending the events.

The efforts at CFM are devoted to achieve mainly three objectives: spreading scientific culture, generating scientific vocation, and including the gender and diversity perspective in all the activities organized, trying to maximize the visibility of our women researchers, ensuring the gender balance in the talks organized, promoting the awareness on the situation, and promoting diversity as the only possible way forward.

Within this spirit, CFM implemented a complete scientific outreach program, and during 2020 more than 28 activities and events were organized, many of them in collaboration with other institutions.

It is worth mentioning that the way we address society has necessarily changed. While adapting to the new dynamics has been a great effort, it has been worthwhile. More than 10 000 people were able to participate in the activities organized in the most challenging year for social relations in history. Thanks to all the volunteers who made it possible and to all the public who supported us by attending the events.

#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.

Given the situation, in 2020 CFM was only able to offer this activity during the months of January and February, hosting the visit of 152 students.

JANUARY	FEBRUARY
Zubiri-Manteo BHI (Donostia / San Sebastián)	**Summa Aldapeta** (Donostia / San Sebastián)
CPES Nazaret Batxilergoa BHIP (Donostia / San Sebastián)	**Urretxu-Zumarraga Ikastola** (Urretxu)

EMAKUMEAK ZIENTZIAN 2020

emakumeakzientzian.eus

7-14/02/2020

CIC nanoGUNE, CIC biomaGUNE, DIPC, Biodonostia, Polymat, Elhuyar, CEIT, TECNUN, and CFM

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.

To commemorate this day, CFM and CIC nanoGUNE co-ordinated the program that brings together the activities of 9 research centers and science-related institutions in the Donostia / San Sebastián area, 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 60 volunteers onboard, the 9 centers joined forces to present a full week program that aimed teenager women, school kids, elder women (above 55), citizens in general and the scientific community.

The commitment of the entities has been set out in a collaboration agreement, signed by all of them. In it, the entities commit themselves, among other things, to make a financial contribution to guarantee the economic support that will allow the implementation of the program, as well as to involve their staff in the development of the programmed activities.

In addition to the financial contributions of the different entities, the initiative obtained the support of the CSIC, FECyT, the Provincial Council of Gipuzkoa and Fomento San Sebastián.

482
Participants

60
Volunteers

9
Entities

51
Impacts in Media

2 881 500
Estimated Audience

16 368,11 €
Contributions

THE "EMAKUMEAK ZIENTZIAN" INITIATIVE WAS RECOGNIZED WITH THE STEAM **EUSKADI** SEAL

The project passed to the first phase of the I STEAM Euskadi Sariak Awards, which made it worthy of receiving the STEAM Euskadi Seal. The Technical Committee of the award was composed by the Department of Education of the Basque Government, the Research Centre for Scientific and Mathematical Education (CRECIM) of the Autonomous University of Barcelona and the Basque Agency for Innovation, Innobasque, which evaluated the 133 submitted applications.

"QUÉ SABEMOS DE..." TALK SERIES

KUTXAKULTUR PLAZA AT TABAKALERA, DONOSTIA / SAN SEBASTIÁN
6, 13, 20 and 27/11/2020

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.*

The format chosen included a limited on-site audience (40 attendees per talk) and a streaming of the series.

This format allowed us to reach unprecedented viewing rates, with more than 4000 views of the talks.

Available at CFM's YouTube channel or scanning this code

- ### Nuevos Coronavirus: Inesperados compañeros de viaje
  Isabel Sola (CNB-CSIC)
  Co-director of the Coronavirus Laboratory of the National Biotechnology Centre, CNB-CSIC

- ### Creando nuevos materiales en la nanoescala
  Martina Corso (CFM)
  CSIC Researcher at the Nanophysics Laboratory at CFM

- ### La frontera de la física fundamental
  Alberto Casas (CSIC-UAM)
  Doctor in Theoretical Physics and Research Professor at the Institute of Theoretical Physics (CSIC-UAM).

- ### Biotecnología con las herramientas CRISPR en los tiempos del coronavirus
  Lluís Montoliu (CNB-CSIC y CIBERER-ISCIII)
  CSIC and CIBERER-Carlos III Health Institute Researcher at the National Biotechnology Centre in Madrid.

PRIDE IN STEAM DAY

orgulloenciencia.dipc.org

ONLINE

18/11/2020

In 2019 the DIPC, CIC nanoGUNE and CFM created the space "Pride in Science" to send a message loud and clear: in science the more diverse, the better. Breaking stereotypes is vital, and to that end, giving visibility to scientists of the LGTBIQA+ collective is fundamental to create new references.

In 2020, CFM together with CIC nanoGUNE and DIPC organized an online meeting with 6 researchers from the LGTBIQA+ community that brought together more than 400 high school students from 10 different schools.

With this initiative, CFM joined the international movement PrideinSTEM (Science, Technology, Engineering, and Mathematics), and the national organization PRISMA.

Available at CFM's YouTube channel or scanning this code

Javier Armentia (Chair)

Juani Bermejo-Vega

Mari Luz Cádiz

Daniel Martínez-Tong

Laura Muelas de Ayala

Marina Peña

LA CIENCIA SEGÚN FORGES

EUREKA! ZIENTZIA MUSEOA, DONOSTIA / SAN SEBASTIÁN
02/12/2020 - 17/01/2021

CFM, in collaboration with Eureka! Zientzia Museoa, presented "Science According to Forges", a unique opportunity to enjoy the exhibition produced by the Spanish National Research Council (CSIC) in homage to the great Antonio Fraguas.

66 vignettes make up an exhibition that has travelled all over Spain and was on display exclusively in the Basque Country, open and free of charge in Eureka! Zientzia Museoa.

More than 2 000 attendees visited the exhibit.

Available at CFM's YouTube channel or scanning this code

OUTREACH TALKS

In addition to the "Que sabemos de..."cycle or the "Emakumeak Zientzian" initiative, two more talks were organized by CFM, and many researchers were invited to participate in several outreach events, listed below:

ORGANIZED BY CFM

The world's smallest car race
Nicolás Lorente (CFM) and Christian Joachim (founder of the NanoCar Race)
29/01/2020
Kutxakultur Plaza (Tabakalera)

El coronavirus y el futuro que nos espera (round table)
Sara de La Rica, Eduardo Maíz y Juan Ignacio Pérez
Chairman: Aitor Bergara
26/09/2020
Bidebarrieta Library

II CURSO DE CULTURA CONTEMPORÁNEA

Las ciencias y las humanidades en la cultura contemporánea
Gustavo Ariel Schwartz
16/10/2020
Online

ZIENTZIAREN GILTZAK
Talks organized by *Zientziaren Giltzak* science community at Ondarroa

Argia ttiki egiten denean
Javier Aizpurua
19/10/2020
Behikozini (Ondarroa)

PRISMA CONFERENCE

Outreach to get out there
Idoia Mugica (CFM)
16/11/2020
Online

ZIENTZIA KUTXA
Talks organized by DIPC and *Kutxa fundazioa*

Supereroankortasuna, markak hausten!
Ion Errea
29/05/2020
Online

CINEMA AND SCIENCE
Cycle organized by DIPC and *Filmoteka Vasca*.
Presentation and discussion on the following movies:

Agora
Pedro Miguel Etxenike
20/01/2020
Tabakalera (Donostia)
11/01/2020
Museum of Fine Arts of Bilbao

Her
Gustavo Ariel Schwartz
06/02/2020
Tabakalera (Donostia)
08/02/2020
Museum of Fine Arts of Bilbao

X: The man with X-Ray eyes
Javier Aizpurua
05/03/2020
Tabakalera (Donostia)
07/03/2020
Museum of Fine Arts of Bilbao

Outreach talk in the framework of the cycle:

Herramientas de luz: de la ciencia ficción a las películas moleculares
Nerea Zabala
26/02/2020
Bidebarrieta Central Library

ACTIVITY IN MASS MEDIA

During 2020, CFM was cited over 300 times in the media, including press, online articles, TV and Radio.

Press articles
46*

Online press
240*

Radio
56

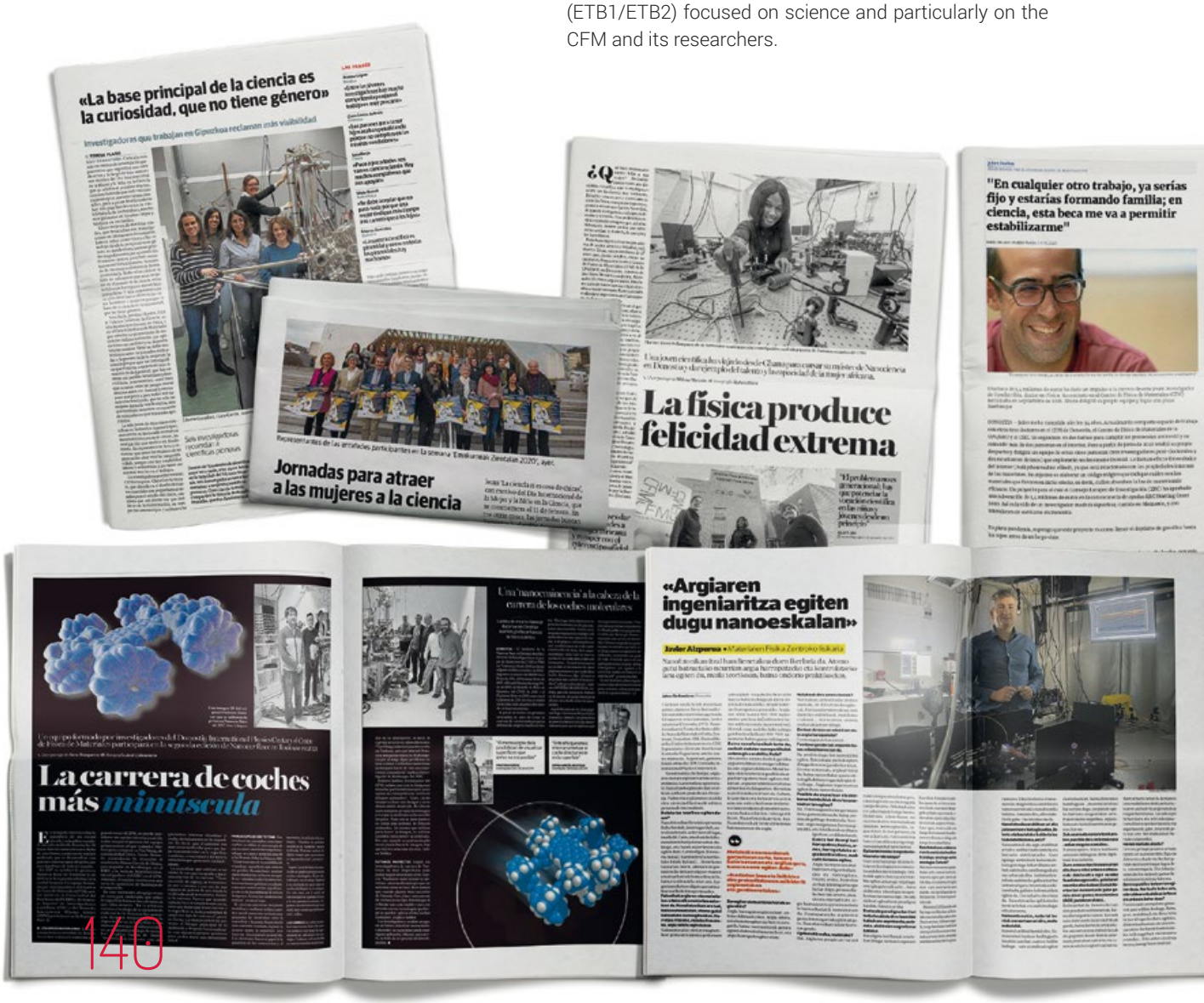
TV
13

*Scientific publications excluded

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.

An example of this intense activity is Ion Errea's collaboration with ***Udako Faktoria*** program that continued throughout the summer on a weekly basis, and the 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. In addition to this, since September 2020 every two weeks Idoia Mugica presents a science section in the daily TV show "Eztabaidan" in the Basque Public Television (ETB1).

Many researchers were invited to participate in debates, interviews or articles in the general press. Television programs such as "Ur Handitan" (ETB1) or "Teknopolis" (ETB1/ETB2) focused on science and particularly on the CFM and its researchers.



@CFMDONOSTIA

CFM is also present and active online and in the social media, and can be officially found in Twitter, Instagram, YouTube and, LinkedIn, as well as in **CFM website**.

As of February 2021, we had more than 1000 followers in Twitter, 243 in Instagram, and 261 in LinkedIn. CFM's YouTube channel already contains more than 30 videos featuring different events. Besides, the CFM website is very regularly updated with news, workshops, seminars, and much more. Our Job Offers section, which is of great interest for many of our visitors receives most of the traffic.

Users can **subscribe to CFM´s mail list** to be updated on the information about the activities and events organized at CFM 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 Center

CIC nanoGUNE

CIC biomaGUNE

Polymat

Biodonostia

Tecnun

Ceit

Elhuyar

Eureka! Zientzia Museoa

Pride in STEM

PRISMA

Pint of Science

Aulas Kutxa – kutxakultur

FECYT

Diputación Foral de Guipúzcoa / Gipuzkoako Foru Aldundia

Fomento-Sustapena Donostia / San Sebastián

La Mecánica del Caracol (Radio Euskadi)

Goiz Kronika eta Udako Faktoria

Eztabaidan

Cátedra de Cultura Científica (UPV/EHU)

GENDER EQUALITY & DIVERSITY AT CFM

Since the need for a specific Gender Equality Plan (GEP) at CFM was first envisioned in 2017, CFM has succeeded in its development and is fully immerse in the implementation of the latter. In this four-year process, it has become clear that a gender plan goes far beyond the goal of achieving parity in the gender balance. It must be an active instrument to guarantee a safe, friendly and attractive work environment for any person, regardless of gender, race, religion or sexual orientation.

The design of the GEP was the result of a collective process. This process was driven by the Gender Equality Committee, formed by staff members representing CFM's different working areas. The Committee remains active in the critical phase of the implementation that will last 4 years. During 2020 Elhuyar, which is approved by Emakunde (the Basque Institute for Women) to give technical Gender Equality support to institutions, has been giving technical advice and supporting CFM in this major task, and continues to do so in 2021.

The current GEC is composed by:

- Daniel Sánchez Portal (Director and Plan's Responsible)
- Idoia Mugica Mendiola (Coordinator)
- Elixabet Sarasketa Zabala
- Arantza Iturrioz Ezeiza
- Nerea Zabala Unzalu
- Gabriel Molina Terriza
- Sara Barja Martínez
- Ester Verde Sesto
- Cristina Mier González
- Amaia González Azpeitia

All the information on the GEP is updated in CFM's webpage. Any researcher can also reach the gender equality committee at any time, and a specific email account regarding equality issues was created to ensure the proper communication with the community.

PLAN IMPLEMENTATION OVERVIEW (2020-2024)

CFM's 1st Gender Equality Plan has a total of 5 key areas, 8 objectives and 44 actions.

KEY AREA	OBJECTIVES	ACTIONS
Organizational culture	• Create an inclusive organizational culture, with a gender-aware leadership and transparency at its core • Promote diversity and inclusivity with the institutional use of language (written and visual)	14
A diverse workforce	• Improve the gender balance at all work-positions and levels • Promote initiatives to support the career progression of the underrepresented gender to high and top positions	11
Work-life balance	• Develop a working environment that facilitates the combination of work, family and private life for women and men	6
Sexual harassment at the working environment	• Prevent and combat sexual and gender-based sexist harassment at CFM.	8
Gender equality and research	• Promote gender-aware research excellency within and outside CFM • Promoting gender diversity and inclusivity at congresses and conferences	5

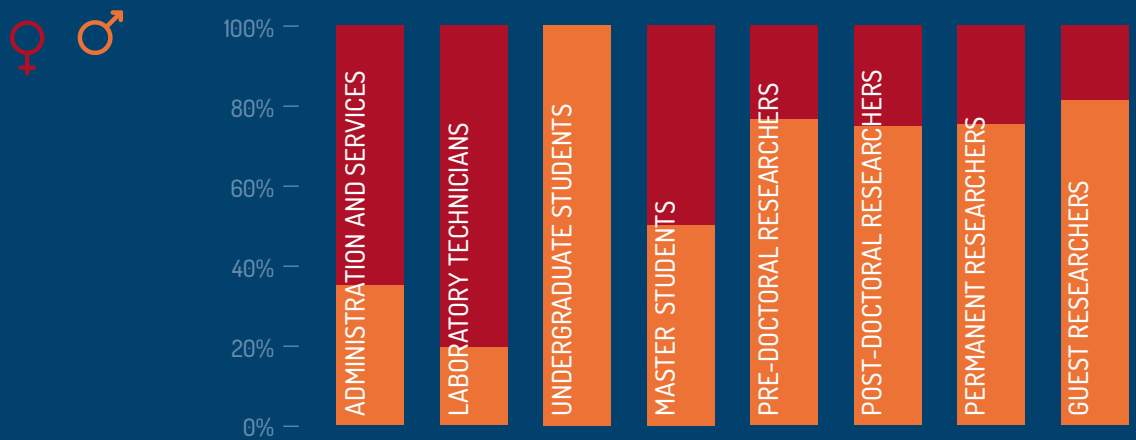
DIAGNOSIS 2020

Looking to raise awareness on the matter, the CFM is committed to run an analysis of the internal situation yearly, publishing the compilation of its own indicators on gender balance. Data of 2020 is presented in the following table and figures:

	♀	♂	
ADMINISTRATION AND SERVICES	9	5	**14**
LABORATORY TECHNICIANS	4	1	**5**
UNDERGRADUATE STUDENTS	0	3	**3**
MASTER STUDENTS	6	6	**12**
PRE-DOCTORAL RESEARCHERS	14	48	**62**
POST-DOCTORAL RESEARCHERS	12	37	**49**
PERMANENT RESEARCHERS	11	35	**46**
GUEST RESEARCHERS	3	14	**17**
	59	149	**208**

CFM is a highly masculinized workforce (71,6% men and 28,4% women at the moment), presenting vertical segregation, with women lacking at top management positions.

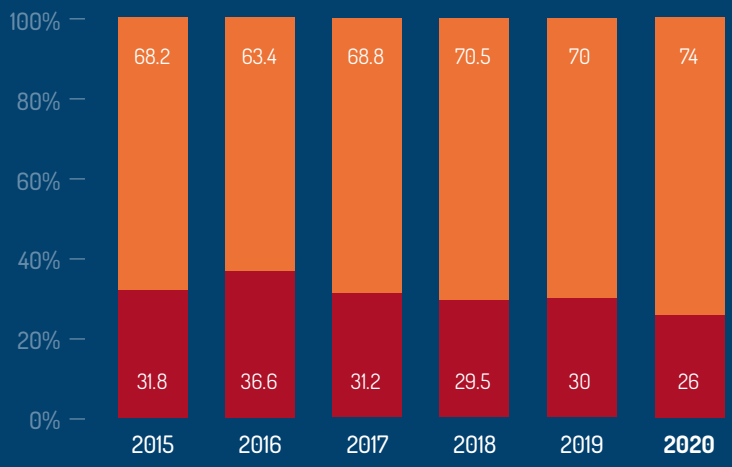
Staff distribution at CFM according to category and gender (percentage)



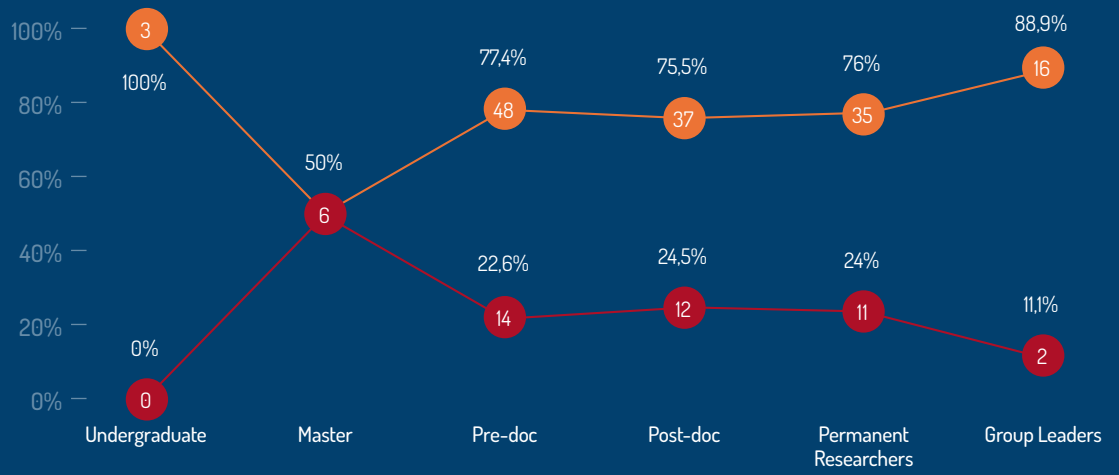
According to this data, the disproportion in the distribution of women/men in the center starts already at the earliest stage of the scientific career. Currently, less than 25% of the pre-doctoral researchers at CFM are women. The gender imbalance is accentuated as the responsibility for the job and level in the research career is greater, corroborating the general trend observed in the Basque Autonomous Community, Spain and Europe.

Regarding the evolution of the gender distribution of CFM scientific staff (including technical staff), since 2017 has remained at a ratio of about 30/70 (women/men), being the 2020 data the worst measured so far.

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



Distribution of CFM Scientific community in percentage by gender and position



CFM scientific staff (including technical staff) has remained at a ratio of about 30/70 (women/men)

ACTIONS IN PLACE 2020

When the CFM GEP was officially launched in October 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 vocation in young women.**

The organization of the "International Day of Women and Girls in Science", and the celebration of the "Pride in Science Day", which have been described in depth in section Science and Society of this report, stand out.

In addition to this programs, 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 for further detail).

Nevertheless, it is worth mentioning that during 2020 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.
- 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", Donostia WeekInn, etc.

MISCELLA-NEOUS

PHD RECRUITMENT FAIR 2020

In 2020 CFM organized the third PhD Recruitment Fair as part of the strategic plan to recruit new talent. From the applications received, 21 applicants were short-listed for online interviews. In the interviews, the candidates had the opportunity to discuss the research projects with the supervisors of the different projects and/or the Evaluation Committee.

After the evaluation, 7 candidates were selected and granted full studentships to join one research group at CFM:

- **Alberto Hijano Mendizabal**
  Group: Mesoscopic Physics
  Supervisor: F. Sebastián Bergeret Sbarbaro
- **Claudia Borredon**
  Group: Polymers and Soft Matter
  Supervisor: Gustavo A. Schwartz Pomeraniec
- **Bruno Josu Diego López**
  Group: Quantum Theory of Materials
  Supervisor: Ion Errea Lope
- **Francisco Javier Manterola Marañón**
  Group: Spectroscopy at Atomic Scale
  Supervisor: Lucia Vitali
- **Alba María Jumbo Nogales**
  Group: Nanomaterials and Spectroscopy
  Supervisor: Yury Rakovich
- **Martin Davide Arena**
  Group: Polymers and Soft Matter
  Supervisor: Josetxo Pomposo Alonso
- **Jonathan Sepúlveda Henríquez**
  Group: Theory of Nanophotonics
  Supervisor: Javier Aizpurua iriazabal

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 three 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 would carry out six-month research stays at DIPC and CFM. The Provincial Council of Gipuzkoa financed each of these long stays with 25 000€. The female African researcher visiting and collaborating at CFM in 2019 and early 2020 was Dr. **Jetro Epse Njukeng Nkengafac** from Cameroon, who joined the Polymers and Soft Matter group, hosted by Prof. Ángel Alegría. However, her stay was interrupted by the health alert caused by COVID19.

Dr. **Aline Simo** from Cameroon was the selected candidate to join Jorge Sánchez Dolado's team at the Ceramic and Cement-Based Materials group of CFM in 2020, but once again, her stay had to be cancelled due to the pandemic emergency.

Unfortunately, Dr. **Aline Simo** will not be able to join the CFM in the end, and it will be Dr. **Mary Ogundiran** from Nigeria who will enjoy this program, hosted by Jorge Sánchez Dolado at the Ceramic and Cement-Based Materials group of CFM. Her stay has been delayed to November 2021.

The next selected candidate of the 2020 call, Dr. **Abeer Adel** from Egypt, is scheduled to start her stay at the end of June 2021. She will join the Polymers and Soft Matter group with Silvina Cerveny as the hostess.

LEARN AFRICA

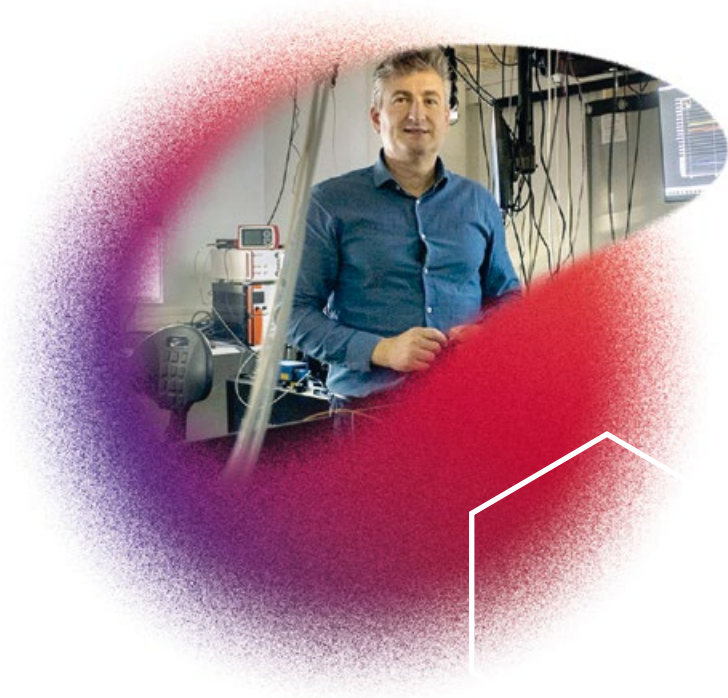
Together with the "Science by Women" program, the Women for Africa Foundation launches "Learn Africa", an initiative that aims to promote the transfer of knowledge, exchange and training of undergraduate and graduate young African women students through scholarships in Spanish universities that collaborate 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 2020, Harriet Kumi from Ghana, the recipient of the scholarship in 2019, finished and defended her Master Thesis at CFM under the supervision of Gabriel Molina at the Quantum Nanophotonics Lab.

HIGHLY CITED RESEARCHER 2020

PROF. JAVIER AIZPURUA IRIAZABAL

After being included for the first time in 2017, Professor Javier Aizpurua remained in the 2020 list of the most cited researchers in the world for the fourth 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.



ERC GRANT FOR THE PHOTONOW PROJECT BY DR. JULEN IBAÑEZ

The European Research Council (ERC) approved a grant of 1.4 million euros to Julen Ibáñez, a researcher from the UPV/EHU at CFM, in the ERC Starting Grant 2020 call for proposals. Thanks to this grant, Dr. Ibañez will be able to create his own research team, giving work to 3 post-doctoral researchers and 2 PhD students, and will also be able to acquire a High Performance Computing (HPC) cluster. It will be a great boost to carry out this research project linked to this unusual photovoltaic effect during the next 5 years.

THE SCIENCE OF CONCRETE THAT COULD WORK THE MIRACLE

The European Commission, within its FET Open program (Future Emerging Technologies), granted over three million euros to the research project MIRACLE (Photonic Metaconcrete with Infrared RAdiative Cooling capacity for Large Energy savings) to design a photonic concrete with autonomous cooling capacity by radiative emission.

The project is led by the researcher Jorge S. Dolado, from the Center for Materials Physics (CFM, mixed center CSIC-UPV/EHU) and has the participation of the Public University of Navarra (UPNA), TECNALIA, the Polytechnic University of Darmstad (TU Darmstad), the Catholic University of Leuven (KU Leuven), Microligh3D, and the Polytechnic University of Turin.

cfm.ehu.es

Paseo Manuel de Lardizabal, 5
E-20018 Donostia / San Sebastián
TEL (+34) 943 018 786

Report Coordination: Idoia Mugica
Edition and corrections: Ioritz Paulis and Idoia Mugica
Photo/Picture credits: Ioritz Paulis and Javier Larrea
Design: batuta.eus