

CFMD
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Materialen Fisika Zentroa
Centro de Física de Materiales
Materials Physics Center

ACTIVITY REPORT

2021

 **CSIC**
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS


Universidad
del País Vasco
Euskal Herriko
Unibertsitatea

MPC-BERC
Materials Physics Center
Basque Center for Materials Research

ACTIVITY REPORT 2021

CFM

Centro de Física de Materiales
Materialen Fisika Zentroa
Materials Physics Center



SUMMARY

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FOREWORD

We would like to thank the good attitude, responsibility and commitment of all CFM's staff that contributed to making these difficult times less hard.



Iñaki Juaristi Oliden, Vicedirector

The year 2021 came with the challenge of adapting to the reality imposed by a pandemic that has given us little respite. One of the consequences of the restrictions was the severe reduction in the number of face-to-face interactions between researchers and staff. Holding meetings, seminars, workshops and courses is a crucial ingredient in the daily life of a research center like CFM, especially for younger researchers and PhD students, who need a more continuous and closer contact with their supervisors and colleagues. That is why CFM facilitated online meetings, teleworking, and allowed the return to direct contact as soon as possible, always guaranteeing everybody's safety with protocols that were made more and more flexible according to the health measures in force. During the last months of 2021, we were also able to start traveling again to attend conferences and visit our colleagues abroad. We would like to thank the good attitude, responsibility and commitment of all CFM's staff that contributed to making these difficult times less hard.

As proof of this, and in spite of all the difficulties, 2021 has once again been a good year from the point of view of the scientific production of CFM, both in quantity and quality, as can be seen in this report. We have again produced over 200 publications, including some in the most prestigious journals in our fields of specialization. It has also been an excellent year for fundraising. To cite a few examples: the ERC Starting Grant PhotoNow started in June 2021, CFM participates in the ERC Synergy Grant Bold and coordinates the FET-OPEN Miracle project that started in February 2021. In total there are 77 projects underway, with close to 4 M€ raised by CFM researchers in 2021 alone. The total rises above 5.1 M€ if we include

the MPC-BERC grant. In addition, 14 doctoral theses have been defended with CFM supervisors. We also keep increasing our technology transfer activity, favoring the creation of collaborations with private companies interested in our research and characterization capabilities.

A very important highlight of 2021 has been the renewal of the distinction as a Basque Excellence Research Center (BERC) of the conglomerate constituted by the CFM (CSIC-UPV/EHU) and the MPC Research Association. The BERC mention, awarded by the Department of Education of the Basque Government, has associated funding of more than 5.5 M€ for the period 2022-2025. Another milestone has been the participation of CFM in the IKUR Strategy also launched by the Department of Education. CFM participates in all four areas covered by the program: Neurobiosciences, Quantum Technologies, High Performance Computing & Artificial Intelligence, and Neutronics. With the support from IKUR, CFM plans to launch new experimental activities in Quantum Technologies and Neurobiosciences. IKUR will also be key to further develop the already powerful lines on Neutron Science research and computer science for Materials Simulations.

During 2021, CFM grew with the incorporation of new researchers. Roberto Robles Rodríguez, a specialist in the theoretical study using ab initio techniques of the electronic and magnetic properties of atoms and molecules on surfaces, joined the Quantum Phenomena on Surfaces group as a CSIC tenured scientist. Armando Maestro Martín joined the Polymers and Soft Matter group as an Ikerbasque Associate Professor. Armando



Daniel Sánchez Portal, Director

2021 has once again been an excellent year in terms of scientific production and fundraising, achieving more than 200 publications and 5.1 M€ in projects.

aims at establishing a new research line to study biological interfaces and bio-inspired interfacial materials using several techniques, including neutron and X-ray scattering. Finally, Julen Ibáñez Azpiroz also joined CFM as an Ikerbasque Associate Professor to develop the ERC Starting Grant PhotoNow, which he obtained on the second-half of 2020. Julen is developing theoretical approaches to study the bulk photovoltaic effect, a non-linear light absorption effect that only occurs in certain special materials and that could be advantageous in harnessing solar energy.

As research groups grow, CFM's administration and core services also need to expand. Thus, during 2021, we had several valuable incorporations, such as Arantza Iturrioz Ezeiza, who permanently joined CFM's R&D Project Management and Technology Transfer office. Recent months have seen the additions of Arkaitz Nagore Ibero, as Responsible for Public Procurement and Administration for the MPC, María José Sánchez Álvarez, as Executive Secretary and contact with the UPV/EHU administration. Finally, Ekain Ugalde Goldarazena joined recently as Maintenance Assistant.

During 2021 several of our colleagues retired after a long and productive academic and research career. Professors Juan Colmenero de León, Eugene Chulkov, Alberto Rivacoba Ochoa and Isabel Tellería Echeverría retired in September 2021. We will greatly miss everyday contact with Alberto and Isabel, and we wish them the best in their new life. Juan Colmenero and Eugene Chulkov will remain at CFM as Emeritus Professors. We feel very fortunate to keep counting on their experience.

One tragic moment in recent months was the extremely serious accident suffered by our colleague Fernando Álvarez González. With these lines, we want to send Fernando and his family our support and wish him a fast and full recovery, which would be the best news that we could expect for the present year.

Besides the several successes already mentioned above, during 2021 we have other reasons to celebrate. Our colleague Sebastián Bergeret Sbarbaro was awarded the Friedrich Wilhelm Bessel Award 2021. The research team behind the EU Fet-OPEN project Engineered ARTificial proteins for Biological Light-Emitting Diodes (ARTIBLED), with our colleague Pedro Braña Coto as the leader of the theory node at CFM, received the 2021 Materials Chemistry Division Horizon Prize (Stephanie L Kwolek Award).

CFM's position at the forefront of research in materials science is only possible thanks to the commitment of all CFM personnel and to the decisive and continuous support of the three key institutions behind CFM: CSIC, UPV/EHU and the Basque Government. We also count on the support from Gipuzkoa Province Government. With these allies we are fully confident that we will maintain our upward trajectory of producing basic science at the highest level and with increasing international visibility.

Thank you all for your commitment and support.

Daniel Sánchez Portal
Iñaki Juaristi Oliden

GOVERNANCE

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 composed of UPV/EHU staff, CSIC staff, as well as Ikerbasque staff.



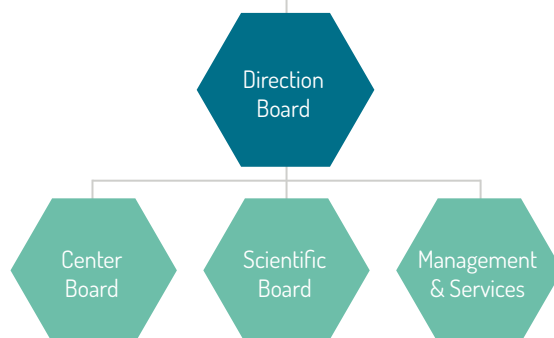
CFM

CSIC

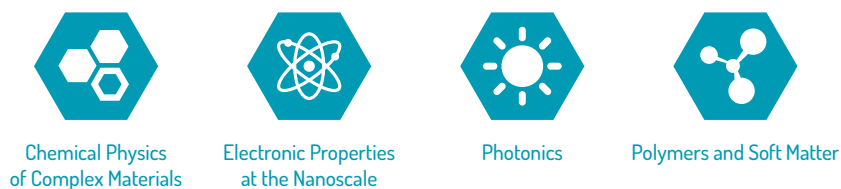
UPV/EHU



Board of Governance



Research Lines



MPC-BERC

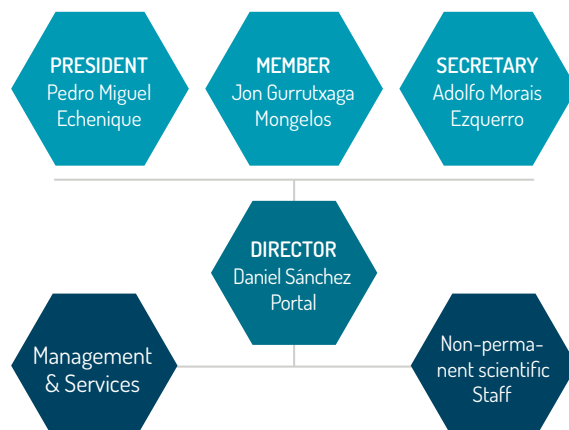
The association “Materials Physics Center” (MPC) is a non-profit organization declared as Basque Excellence Research Center (BERC) which is intrinsically united to CFM, and shares its goals and scientific activity, serving as an instrumental body in a totally synergistic and combined activity. The body 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.

MPC – BERC

DIPC

Gipuzkoako Foru Aldundia

Ikerbasque



PROFILE

SCIENTIFIC COMMUNITY

Researchers in
Action

223

18

Research Groups

TRAINING

14

PhD Theses
defended

18

Master Theses
Defended¹

8

Undergraduate
Projects

RESEARCH OUTPUT

ISI Publications

216

Q1 Publications

WOS: 59%
SCOPUS: 86%

D1 Publications

WOS: 29%
SCOPUS: 41%

Citations²

14778

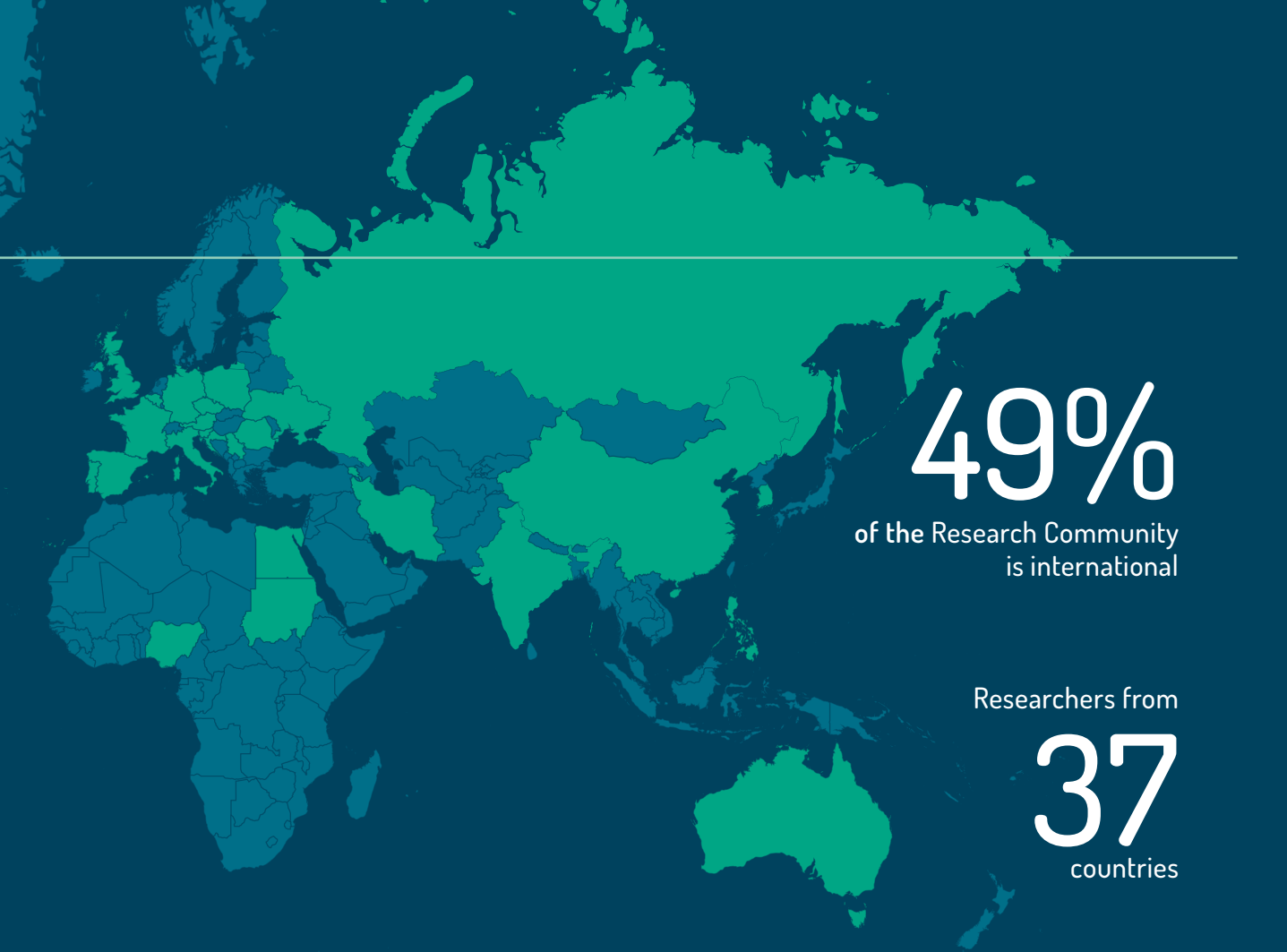
H Index

143

International Collaborations

82%

10



49%
of the Research Community
is international

Researchers from
37
countries

ACTIVITIES AND EVENTS

Conferences, Workshops,
Courses, and Seminars

14

Science and Society

+60 Activities

+9000 Attendees

PROJECTS AND FUNDING

Ongoing Projects

77

Funding

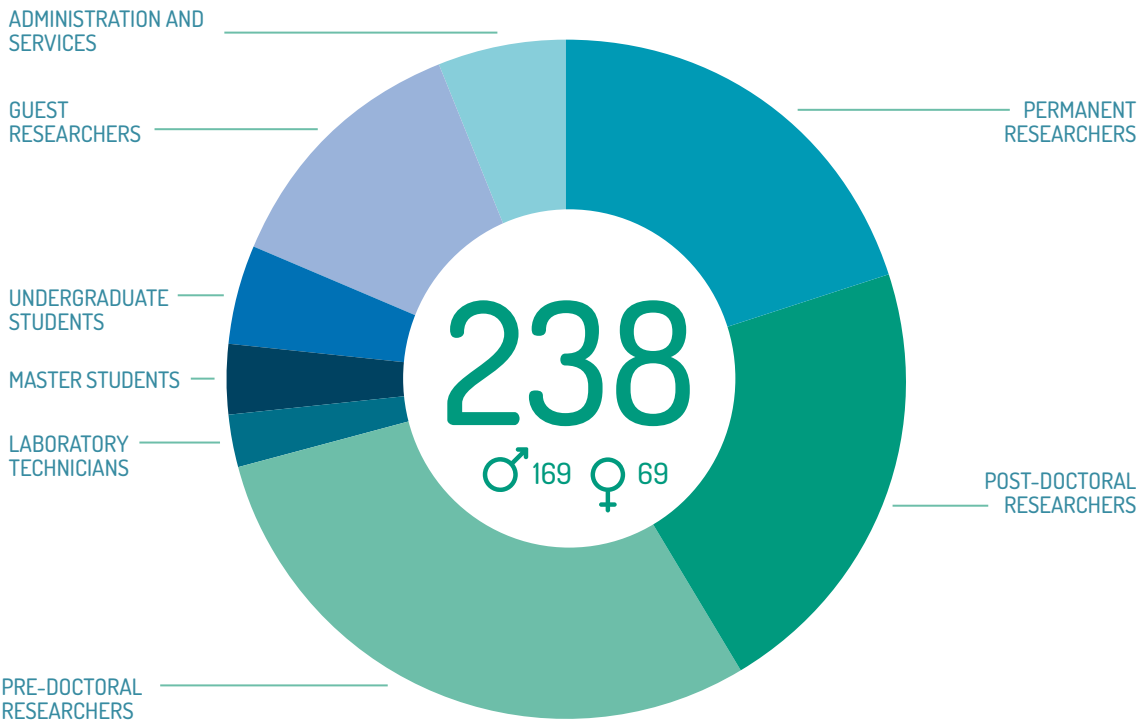
5 131 085,42 €

¹ In the framework of the nanoscience master or supervised by CFM staff

² Including Physical Review B: 81%

PEOPLE

ALL THE CFM COMMUNITY



CFM Staff

197

Researchers in Action

223³

Permanent Researchers	48
Post-doctoral Researchers	51
Pre-doctoral Researchers	70
Laboratory Technicians	6
Master students ¹	8
Undergraduate students ²	11
Guest Researchers	30
Administration and Services	14
Total	238

¹ Two of those receive scholarships during their stay at CFM and are considered staff

² Six of those receive scholarships during their stay at CFM and are considered staff

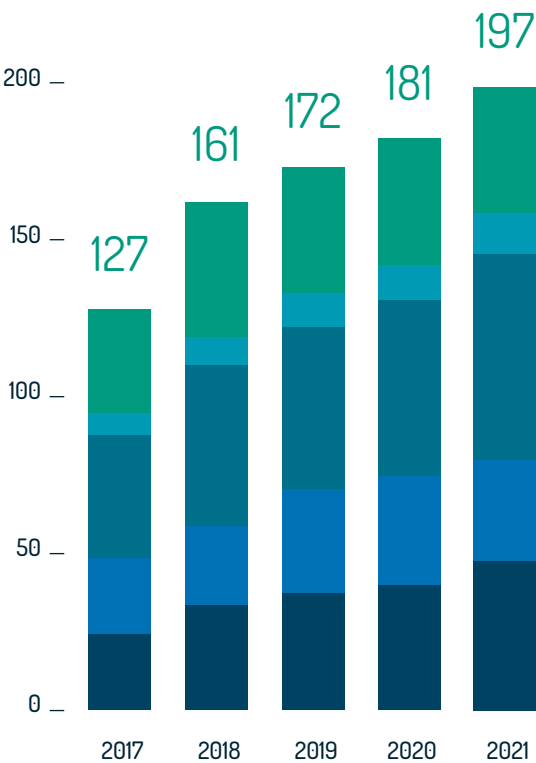
³ Including Guest researchers, undergraduate and master students

DISTRIBUTION OF CFM STAFF

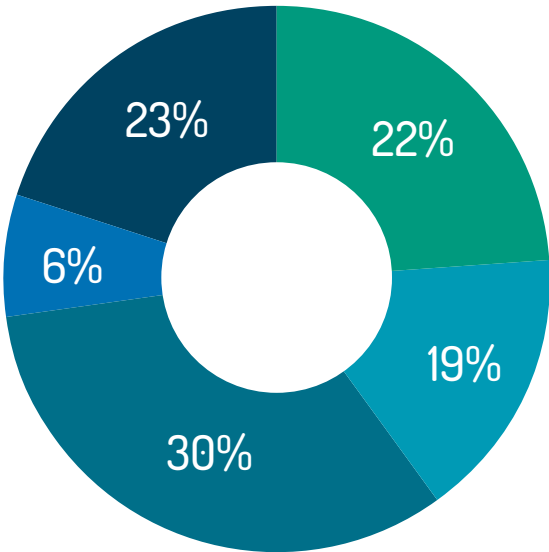
according to the origin of the financial support

	2017	2018	2019	2020	2021
CSIC	24	33	37	40	47
UPV/EHU	24	25	33	34	32
MPC-BERC	39	51	51	56	65
IKERBASQUE	7	9	11	11	13
COLLABORATORS	33	43	40	40	40
Total	127	161	172	181	197

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 2021



DIRECTION BOARD

Director: Daniel Sánchez Portal

General Manager: Amaia González Azpeitia

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

Laura Alfonso Zarra, [Administrative](#), MPC

María Formoso Ferreiro, [Administrative](#), MPC

Marta López Pérez, [Administrative](#), MPC

Txema Ramos Fernandez, [Administrative](#), CSIC



Computing and IT Services

Aimar Mindegia Zaldúa, [IT Systems Internship](#), MPC

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

Laura Isabel Fernández Gómez-Recuero, 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 Oriden, *Associate Professor*, UPV/EHU

Maite Alducin Ochoa, *Tenured Scientist*, CSIC

Ricardo Díez Muiño, *Research Scientist*, CSIC

Post-doctoral Researchers

Alberto Pablo Sánchez Muzas

Raúl Bombin Escudero

Pre-doctoral Researchers

Alfredo Serrano Jiménez

Auguste Tetenoire

Ivan Zugec

Undergraduate Student

Iñaki Fernández Tena

Guest Researcher

Heriberto Fabio Busnengo, *Senior Scientist*

02 Quantum Phenomena on Surfaces

Permanent Researcher

Nicolás Lorente Palacios, *Research Scientist*, CSIC

Ikerbasque Fellow

Deungjang Choi, *MPC*

Post-doctoral Researcher

Roberto Robles Rodríguez

Pre-doctoral Researchers

Cristina Mier González

Divya Jyoti

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
Maidor Ormaza Saezmiera, [Associate Professor](#), UPV/EHU
Martina Corso, [Tenured Scientist](#), CSIC

Ramon y Cajal Researcher

Sara Barja Martínez

Post-doctoral Researchers

Andrew P. Weber
Jan Patrick Calupitan
John Fredy Vélez Santa
Khadiza Ali
Marco Gobbi ([Ikerbasque fellow on leave at CIC nanoGUNE](#))
Maxim Ilin
Rishav Harsh
Sabine Auras
Tao Wang
Vahagn Mkhitaryan

Pre-doctoral Researchers

Alaa Mohammed Idris Bakhit
Andrea Aguirre Baños
Carmen González Orellana
Fernando García Martínez
Marina Peña Díaz
Niklas Jonas Friedrich
Paula Angulo Portugal
Rodrigo Castrillo Boderó

Master Student

Francisco Romero Lara

Guest Researchers

Afaf El-Sayed, [Senior Scientist](#)
Amitayush Jha Thakur, [Pre-doctoral Researcher](#)
Andrey Ilin Moskalenko, [Pre-doctoral Researcher](#)
Federico Frezza, [Pre-doctoral Researcher](#)
Ignacio Piquero Zulaica, [Post-doctoral Researcher](#)
Kevin García Díez, [Master Student](#)
Lorena Glatthaar, [Undergraduate Student](#)

04 Modelisation and Simulation

Permanent Researchers

Andrés Arnau Pino, [University Professor](#), UPV/EHU
Daniel Sánchez Portal, [Research Professor](#), CSIC

Post-doctoral Researchers

Mikhail Otrokov

Pre-doctoral Researchers

Joseba Goikoetxea Perez

Malen Etxeberria Etxaniz
Masoud Mansouri
Sophie Espert

Guest Researchers

Krzysztof Michal Czajkowski, [Pre-doctoral Researcher](#)
María Blanco Rey, [Senior Scientist](#)

05 Spectroscopy at Atomic Scale

Permanent Researcher

Lucia Vitali, [Ikerbasque Professor](#), UPV/EHU

Post-doctoral Researcher

Ana Barragán Durán

Pre-doctoral Researcher

Francisco Javier Manterola Marañón

06 Theoretical and Computational Chemistry

Permanent Researcher

Pedro Braña Coto, [Research Scientist](#), CSIC

Post-doctoral Researchers

Giulia Biffi
Stefano Sansotta

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

Rodrigo Humberto Aguilera del Toro

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 Researchers

Djordje Dangic

Raffaello Bianco

Yuewen Fang

Pre-doctoral Researchers

Antonella Meninno

Francesco Belli

Iñigo Robredo Magro

Josu Diego López

Martín Gutiérrez Amigo

Oscar Rodríguez Ballesteros

Guest Researchers

Adolfo Otero Fumega, [Pre-doctoral Researcher](#)

Jonas Bekaert, [Post-doctoral Researcher](#)

09 Mesoscopic Physics

Permanent Researcher

F. Sebastián Bergeret Sbarbaro, [Tenured Scientist, CSIC](#)

Ikerbasque Associate

Vitaly Golovach, [UPV/EHU](#)

Post-doctoral Researcher

Stefan Ilic

Pre-doctoral Researchers

Alberto Hijano Mendizabal

Cristina Sanz Fernández

Jon Ortuzar Andrés

Mikel Rouco Martin

10 Nano-Bio Spectroscopy

Permanent Researcher

Ángel Rubio Secades, [University Professor, UPV/EHU](#)

11 Souza Research Group

Permanent Researchers

Ivo Souza, [Ikerbasque Professor](#), UPV/EHU

Julen Ibañez Azpiroz, [Ikerbasque Associate](#), MPC

Post-doctoral Researcher

Jyoti Krishna

Peio García Goiricelaya

Pre-doctoral Researcher

Álvaro Ruiz Puente

Guest Researcher

Cheol-Hwan Park, [Senior Scientist](#), DIPC

Jose Luis Martins, [Senior Scientist](#)

Liu Xiaoxiong, [Pre-doctoral Researcher](#)

Stepan Tsirkin, [Post-doctoral Researcher](#)

Tomas Rauch, [Post-doctoral Researcher](#)

12 Ceramic and Cement-Based Materials

Permanent Researcher

Jorge Sánchez-Dolado, [Tenured Scientist](#), CSIC

Post-doctoral Researcher

Antoine Patt

Guido Goracci

Pre-doctoral Researchers

Ebtisam Tarek Mohammed Saeed

Mohamad Barzegar

Mohammad Rahjoo

Guest Researchers

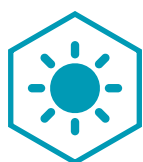
Chokri Lluçia, [Undergraduate Student](#)

Mary Bosede Ogundiran, [Senior Scientist](#)

Miguel Beruete, [Senior Scientist](#)

Matteo Cagnoni, [Post-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

Mario Zapata Herrera

Roberto Álvarez Boto

Sofia Isabel de Carvalho Ribeiro

Pre-doctoral Researchers

Adrián Juan Delgado

Alvaro Nodar Villa

Antton Babaze Aizpurua

Bruno Candelas Peñalba

Carlos Maciel Escudero

Jonathan Antonio Sepúlveda Henríquez

Undergraduate Student

Xabier Arrieta Aristi

Guest Researchers

Elise Prin, [Master Student](#)

Jeremy Baumberg, [Post-doctoral Researcher](#)

14 Nanomaterials and Spectroscopy

Permanent Researchers

Yuri Rakovich, [Ikerbasque Professor](#), UPV/EHU

Marek Grzelczak, [Research Scientist](#), CSIC

Post-doctoral Researchers

María Sanromán Iglesias

Victor Krivenkov

Pre-doctoral Researchers

Alba María Jumbo Nogales

Joscha Kruse

Sara Luisa Marina Barbier

Zuzanna Lawera

Master Student

Xabier Belaunzaran Sanz

Guest Researchers

Aimar Marauri Iriberrí, [Undergraduate Student](#)

Nina Tarnowicz-Staniak, [Pre-doctoral Researcher](#)

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

Rubén Pellicer Guridi

Pre-doctoral Researchers

Iker Gómez Vilorio

Jon Lasa Alonso

Martin Molezuelas Ferreras

Miriam Martínez Flórez

Undergraduate Student

Joseba Solozabal Aldalur

Guest Researcher

Garikoitz Agirre Soto

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 Associate

Armando Maestro Martín

Ikerbasque Fellows

Jon Maiz Sancho, [MPC](#)

Paula Malo de Molina Hernández, [MPC](#)

Post-doctoral Researchers

Daniel Enrique Martínez Tong
Jorge Humberto Melillo
José Ángel Martínez González
María Ester Verde Sesto
Mohammad Ali Aboudzadeh Barihi
Mounika Gosika
Soheil Sharifi
Valerio Di Lisio

Pre-doctoral Researchers

Agustín Blazquez Martín
Amaia Matanza Corro
Carlo Andrea Pagnacco
Claudia Borredon
Davide Arena
Francesco Coin
Javier Martínez Sabando
Jokin Pinacho Olaciregui
Julen de la Cuesta Leone
Maiara Aime Iriarte Alonso
Mariarita Paciolla
Matteo Sanviti
Mohammed El Amine Hanifa
Numera Shafqat

Undergraduate Students

Ainara Ruiz Bardillo
Yanire López Campos
Eric Gómez Urreizti

Guest Researchers

Abeer M. Adel Mohamed Amdelbaky Elbasuony, Senior Scientist
Ana María Stan, Master Student
Ane Izaskun Aranburu Leiva, Pre-doctoral Researcher
Christopher Garvey, Senior Scientist
Claudio Magnani, Master Student
Juan Manuel Garzón Vela, Undergraduate Student
Laura Álvarez Francés, Post-doctoral Researcher
Lorenzo Augusto Rocchi, Undergraduate Student
Mattia Gaboardi, Senior Scientist
Mikel Iguaran Aguirregomezorta, Undergraduate Student
Nicolas Illy, Senior Scientist
Nicolas Uguen, Pre-doctoral Researcher
Nicolás Torasso, Pre-doctoral Researcher
William Coffy, Pre-doctoral Researcher

18 Quantum Beams and Sustainable Materials

Permanent Researcher

Felix Fernández Alonso, [Ikerbasque Professor, MPC](#)

Post-doctoral Researcher

Kacper Druzicki

Pre-doctoral Researcher

Balthasar Braunewell
Pelayo Marín Villa

Guest Researcher

Mohammed Ali Al Assiri, [Master Student](#)

OTHER POSITIONS

Associate Professor

Isabel Tellería Echeverría, [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 Researcher

Wen Wan, [DIPC \(Miguel Moreno's group\)](#)

Pre-doctoral Researchers

Alejandro Berdonces Layunta, [DIPC \(Dimas García de Oteyza's group\)](#)
Miguel Ángel Jiménez Herrera, [MPC \(Dario Bercioux's group\)](#)
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 \(Miguel Moreno's group\)](#)



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.



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 "Modélisation 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.

1

Gas/Solid Interfaces

Group Leader: Ricardo Díez Muiño
Research Scientist CSIC



The "Gas/Solid Interfaces" group focuses on the atom-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 cal-

culations 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. The group applies the synthesis of atomically perfect materials to practi-

cal problems of technological and industrial interest, aligned with three current social challenges: quantum technologies, molecular precision chemical sensors, and catalysts for green energies.

The NPL holds some of the most complete and modern set of highly sensitive surface science techniques, combined with the tools for the growth of materials and nanostructures, from layer-by-layer growth to device fabrication. Thus, NPL laboratory has several multi-technique ultra-vacuum equipment 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 focus 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.

Five theoretical and one experimental 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.

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) nano-

structures, such as graphene and 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



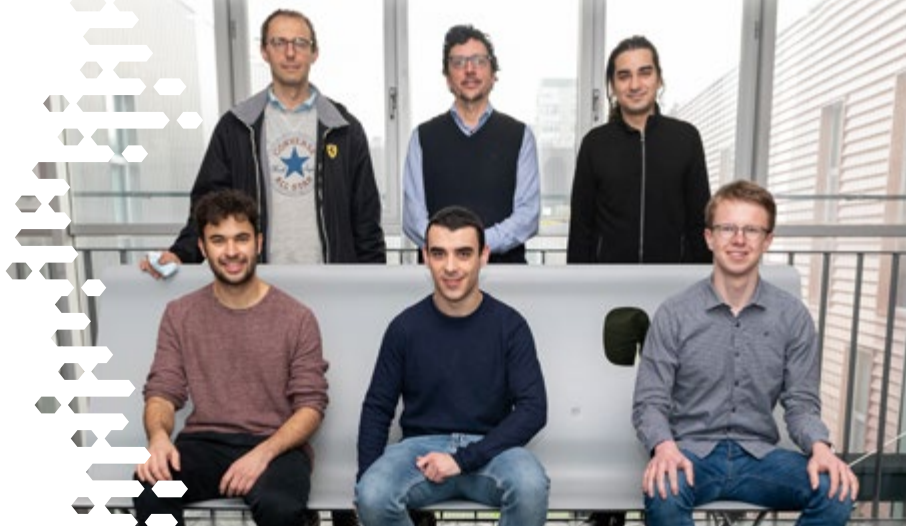
The activity of the “Quantum Theory of Materials” group focuses on the first-principles calculation of materials properties and the development of new ab initio techniques. The group develops new theoretical methods to overcome the problems associated to standard theoretical approaches, specially, to 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; (iv) phonon polaritons; (v) optical lattices; and, finally, (vi) biophysical systems.

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 also been 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 CO₂ fingerprint.

The initial objectives of the group are: (i) the use of atomistic and colloidal simulations to study the struc-

ture 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 vitroceraamics 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. The “Quantum Beams and Sustainable Materials” group (18) complements 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, and 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 dy-

namics 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

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Photoinduced desorption dynamics of CO from Pd(111): A neural network approach

Alfredo Serrano Jiménez, Alberto P. Sánchez Muzas, Yaolong Zhang, Juraj Ovčar, Bin Jiang, Ivor Lončarić, J. Iñaki Juaristi, and Maite Alducin.

Journal of Chemical Theory and Computation 17, 4648 (2021)

Using the Embedded Atom Neural Network (EANN) Serrano-Jiménez *et al.* develop an accurate and extremely complex Potential Energy Surface (PES) that allows a detailed and reliable description of the photo-induced desorption of CO from Pd(111). The obtained EANN-PES is able to describe an extensive range of surface temperatures (90–1000 K), a large amount of degrees of freedom, and the varying CO coverage caused by the abundant desorption events.

Irradiation of an adsorbate-covered metal surface with femtosecond laser pulses, from the near-infrared to the ultraviolet regime, generates a transient nonequilibrium distribution of hot electrons and a subsequent excitation of the lattice atoms via electron-phonon coupling.

As a result, adsorbates encounter a combined electronic and phononic excited system from which they can gain energy, facilitating the initial vibrational excitation, the subsequent diffusion on the surface, and the final recombinative desorption. Usually, the cross-sections for some of these photo-induced reactions are significantly increased respect to what it is observed under ordinary thermal excitation conditions.

From the theoretical side, the modelling of these experiments requires to perform multidimensional Molecular Dynamics (MD) simulations involving multiple adsorbates and surface atoms in the presence of nonequilibrium distributions of excited electrons and phonons. Only very recently this complete description of the problem has been achieved by means of the *ab initio* molecular dynamics with electronic friction and thermostats [(T_e, T_l)-AIMDEF] model [M. Alducin *et al.* PRL 123, 246802 (2019)].

However, the extremely computationally demanding (T_e, T_l)-AIMDEF methodology severely limits the achieved statistics, the simulation time, and the size of the system to model. These limitations could nowadays be overcome if it were possible to construct a multidimensional potential energy surface of *ab initio* quality, from which the atomic forces could be rapidly, but accurately, calcu-

lated. In principle, multidimensional potential energy surfaces can be generated using Neural Networks (NN-PES). However, the requirements imposed to a NN-PES capable of describing femtosecond laser induced reactions are unprecedentedly extreme and demanding due to the necessity of modeling the movement of multiple adsorbates and great number surface atoms under an ample range of varying lattice and electronic temperatures.

In this work, the authors demonstrate that the new embedded atom neural network method [Y. Zhang *et al.* **J. Phys. Chem. Lett.** **10**, 4962 (2019)] allows to develop

such accurate and extremely complex NN-PES for the specific case of the description of the photo-induced desorption of CO from the Pd(111) surface with a coverage of 0.75 monolayers. MD simulations performed in this NN-PES reproduce with great accuracy the *ab initio* molecular dynamics simulations. Moreover, the presented methodology is completely general and can be applied to any other adsorbate-surface system and different coverages. For all these reasons, it opens the path to, from a theoretical point of view, fully characterize and understand the femtosecond laser pulse induced chemistry at surfaces.

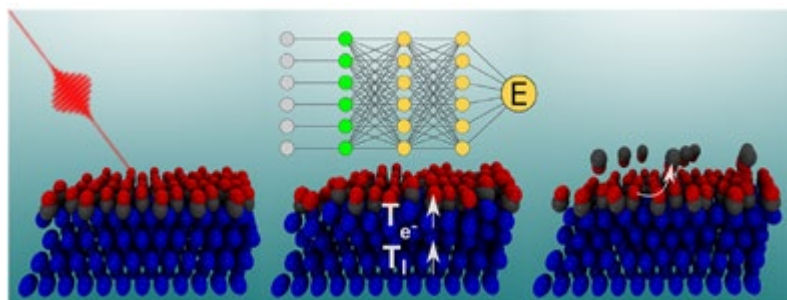


Figure: Scheme of the photo-induced desorption of CO from Pd(111) with a coverage of 0.75ML. Molecular dynamics simulations are performed using a Multi-Dimensional Neural Network Potential Energy Surface that reliably describes highly varying surface temperatures (90-1000 K) and CO coverages (0.33-0.75 ML).

Atomically-precise texturing of hexagonal boron nitride nanostripes

Khadiza Ali, Laura Fernández, Mohammad A. Kherelden, Anna A. Makarova, Igor Piš, Federica Bondino, James Lawrence, Dimas G. de Oteyza, Dmitry Yu. Usachov, Denis V. Vyalikh, F. Javier García de Abajo, Zakaria M. Abd El-Fattah, J. Enrique Ortega, and Frederik Schiller.

Advance Science 8, 2101455 (2021)

Monolayer hexagonal boron nitride (hBN) can be epitaxially grown on vicinal rhodium (Rh) surfaces using a Rh curved crystal for a systematic exploration, which produces a periodically textured, nanostriped hBN carpet that coats Rh(111)-oriented terraces and lattice-matched Rh(337) facets with tunable width. The electronic structure reveals a nanoscale periodic modulation of the hBN atomic potential that leads to an effective lateral semiconductor multi-stripe.

Since the discovery of graphene, a wide diversity of atomic-layer-thick, two-dimensional (2D) materials with varied properties have emerged. Of particular interest are those that exhibit semiconducting behavior, such as hexagonal boron nitride (hBN). hBN is isoelectronic to graphene and has also a honeycomb lattice formed by alternating nitrogen and boron atoms, but in contrast to the semimetallic graphene, its band structure presents some characteristics that makes it particularly attractive for applications in microelectronics, either alone or in combination with other 2D materials, such as



Featured on the cover of Advanced Science, the STM image and a model of how hBN covers a cylindrical Rh crystal approx. 10° away from the (111) direction.

graphene. Furthermore, hBN is structurally robust and chemically inert. Although hBN flakes may be obtained by mechanical exfoliation of bulk crystals, a single hBN monolayer can be readily synthesized on metal surfaces, leading to structurally and chemically robust substrates that frequently exhibit nanoscale patterns. This makes

hBN-covered metals excellent platforms to achieve functional interfaces with atoms, molecules, and aggregates, as well as to develop hybrid 2D materials, such as twisted Van der Waals stacks or 2D heterostructures. The latter hold a great potential for atomically thin circuitry, such as superstructures formed with isostructural graphene, which are optimal to engineer gaps and doping, as well as to tune and enhance spin scattering.

However, this is easier said than done. Exploiting fine hBN-based nanostructures requires structural quality down to the atomic scale and precise lateral nano-structuration and integration with other two-dimensional materials, which lies beyond current lithographic

“Hexagonal boron nitride nanostripes can be grown on vicinal rhodium surfaces.”

capabilities. The bottom-up vapor growth is the alternative, which also works for 2D hybrids, although general procedures to control shape, size, and spatial order of surface phases are still lacking.

Now, a team of researchers from CFM and other collaborating institutions has found a working disruptive approach: imprinting the lateral pattern of an atomically stepped one-dimensional template into a hBN monolayer. The researchers demonstrate the bottom-up synthesis of nanostriped hBN heterostructures with atomically sharp interfaces. The idea was to follow the standard chemical vapor deposition growth route, using rhodium (Rh) vicinal surfaces as one-dimensional (1D) templates. In practice, hBN was epitaxially grown on Rh surfaces using an Rh curved crystal for a systematic exploration, which produces a periodically textured, nanostriped hBN carpet that coats Rh(111)-oriented terraces and lattice-matched Rh(337) facets with tunable width.

Thus, a 1D lateral hBN (111)/(337) heterostructure arises, featuring defect-free boundaries and significant band offsets. The resulting electronic structure reveals a nanoscale periodic modulation of the hBN atomic potential that leads to an effective lateral semiconductor multi-stripe.

Since size tunability of phases can be gained by selecting the Rh vicinal plane, a variety of new possibilities is opened by this discovery. For example, the hBN (111)/(337) faceted system could be used as a model platform to mold and probe 1D phonon–polariton excitations in the THz regime to achieve selective growth of atoms, aggregates, and molecular adsorbates for organic optoelectronics and catalysis, or to tailor the 3D stacking with other 2D materials, such as graphene.

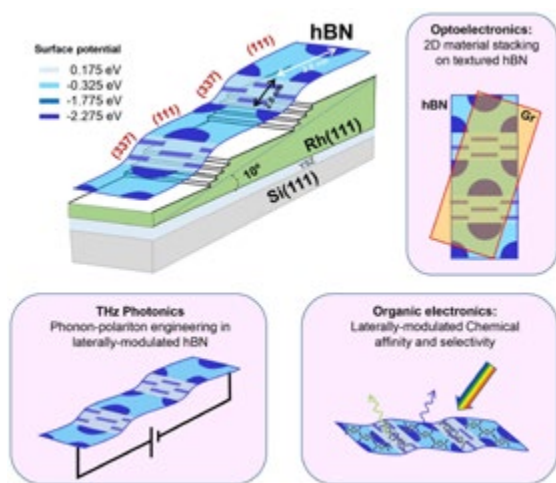


Figure: Lateral nanopatterning of hBN through epitaxial growth. The concept of the study of vicinal hBN/Rh interfaces is presented. CVD growth of hBN induces periodic (111)/(337) faceting of the Rh substrate. The hBN monolayer uniformly coats the faceted substrate, defining an effective lateral hBN/Rh heterointerface with periodic surface potential texturing. Using commercial Rh(111) films, one could exploit such chemical and electronic modulation of hBN to explore phonon–polariton THz excitations, selective growth of optically-active molecules, and vertical stacking with other 2D materials.

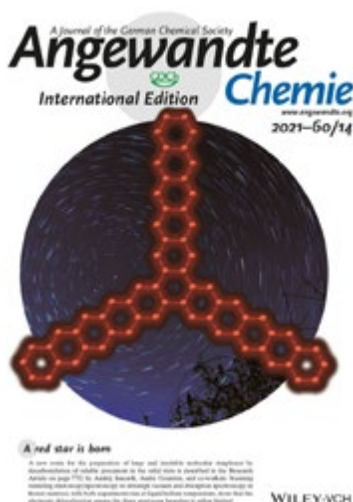
A red star is born

Jan Holec, Beatrice Cogliati, James Lawrence, Alejandro Berdonces-Layunta, Pablo Herrero, Yuuya Nagata, Marzena Banasiewicz, Boleslaw Kozankiewicz, Martina Corso, Dimas G. de Oteyza, Andrej Jancarik, and Andre Gourdon.

Angewandte Chemie International Edition 60, 7752 (2021)

Starphenes are two-dimensional polyaromatic hydrocarbons (PAHs) made up of three acene arms connected via a benzene ring. The foreseen use of starphenes ranges from optoelectronic applications as components in Organic Field-Effect Transistors (OFETs) or Organic Light-Emitting Diodes (OLEDs), to logic gates in single-molecule electronics. Still, starphenes did not reach real applications yet due to their challenging synthesis. In fact, their tendency to interact via π - π stacking make them highly insoluble and only starphenes modified with side groups have been synthesized so far.

In this collaborative work between researchers from different European and Japanese institutions, the largest unsubstituted starphene that has been ever synthesized is reported, namely: the planar and fully conjugated [16]-starphene featuring three penta-cene arms. The chemical strategy employed makes use of carbonyl protecting groups that are easily removed by thermal annealing, ultimately leading to pristine solid starphenes. The large quantities that can be obtained by this new synthetic route pave the way for implementing large starphenes in optoelectronic devices.



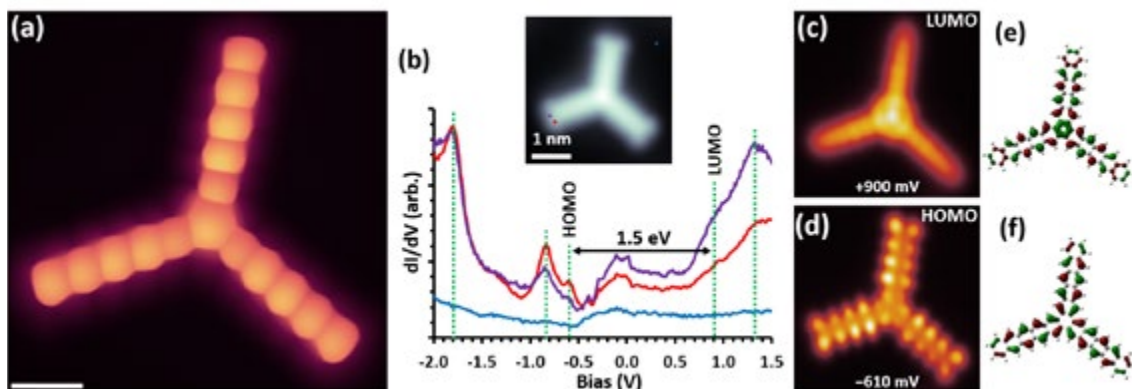


Figure: (a) HR-STM image taken with CO functionalized STM tip that reveals the chemical structure of a single starphene molecule. Scale bar: 5 Å. (b) Differential conductance (dI/dV) spectra measured on a starphene arm showing various resonances marked with dashed lines. The inset marks the positions at which each of the spectra are taken, two on the molecule and one on the substrate as reference. (c) and (d) Constant height dI/dV images of the same starphene recorded with a Cl-functionalized STM tip at the energy of the lowest unoccupied (LUMO) and highest occupied (HOMO) molecular states, respectively. All STM images were recorded at 4.3 K. (e) Calculated LUMO and (f) HOMO of starphene.

The researchers characterized in detailed ensemble starphene properties with a combination of analytic techniques. The CFM team employed an Atomic Layer Injection (ALI) technique for the first time to deposit such large and fragile molecules dissolved in an acetonitrile solution onto a clean metallic surface and succeeded in studying the electronic properties of single starphene molecules by

high-resolution Scanning Tunneling Microscopy (STM). In agreement with theory, starphene exhibits a bandgap (1.64 eV) smaller than pentacene (2.2 eV) and more similar to hexacene (1.76 eV). This implies an enhanced electron delocalization with respect to pentacene. That is, the molecule does not behave as three isolated pentacene arms, but with an electronic coupling between the three arms.

Large perpendicular magnetic anisotropy in nanometer-thick epitaxial graphene/Co/heavy metal heterostructures for spin-orbitronics devices

María Blanco-Rey, Paolo Perna, Adrian Gudin, Jose Manuel Diez, Alberto Anadón, Pablo Olle-ros-Rodríguez, Leticia de Melo Costa, Manuel Valvidares, Pierluigi Gargiani, Alejandra Guedeja-Marron, Mariona Cabero, María Varela, Carlos García-Fernández, Mikhail M. Otrokov, Julio Camarero, Rodolfo Miranda, Andrés Arnau, and Jorge I. Cerdá.

ACS Applied Nano Materials 4, 4398 (2021)

A combination of theoretical modeling and experiments reveals the origin of perpendicular magnetic anisotropy (PMA) in graphene/Co/heavy metal (Pt and Ir) multilayer heterostructures and explains its behavior as a function of the Co thickness. The large experimental critical thicknesses sustaining PMA can only be retrieved in the authors calculations by the inclusion of stacking defects. They find that these defects promote a local hcp stacking, such as twin boundaries or stacking faults that, indeed, are observed in high resolution STEM images.

Understanding the ultimate reasons why Perpendicular Magnetic Anisotropy (PMA) prevails in real multilayer heterostructures is of utmost importance for advancing in the design and development of fabrication processes of spintronic and spinorbitronic devices, e.g., race track memories based on magnetic domain walls or skyrmion motion. In this context, it is instrumental to bridge the gap between the nano- and micro-scales, typically found between state-of-the-art first-principles calculations for ideal systems and the real size of the grown multilayer heterostructures, respectively. This represents a tremendous challenge, because it is precisely in the transition region between these two scales where a delicate balance between quantum-sized effects and the appearance of structural defects determines the properties of the real system.

In this work, the researchers have used a recently developed technique to grow heavy metal/cobalt/graphene multilayer heterostructures. There, the cobalt (Co) planes follow a fct-stacking (fct stands for fcc with lateral tensile strain) and show a reduced number of defects. The evo-

lution of the magnetic properties with Co thickness has been characterized by state-of-the-art techniques, such as Magneto Optic Kerr Effect (MOKE) and X-ray Magnetic Circular Dichroism (XMCD). Both on Pt(111) and Ir(111), these multilayered heterostructures show PMA at unexpectedly large Co thickness; above 20 Co monolayers in the case of Pt(111) buffer layers. Remarkably, we have also unraveled the origin of this observation identifying stacking defects, actually observed in our high-resolution electron microscopy images as the main factor sustaining the PMA at such unusually large thicknesses.

In brief, and although it looks counterintuitive at first glance, the authors found that the presence of locally hcp stacked Co layers, due to stacking faults or twin boundaries, incorporates a further interface in the Co film, which leads to a remarkably large contribution to the PMA. Additionally, thanks to the performed first-principles calculations they were able to quantify the interfacial contributions to the orbital moment anisotropies, finding a surprisingly large value for the Co/graphene interface.

“Our dear friend and colleague Jorge Iribas Cerdá was the driving force of this project but he suddenly passed away too early on June 16, 2021. Therefore, this work represents part of his legacy to the scientific community and we would like to dedicate it to his memory.”

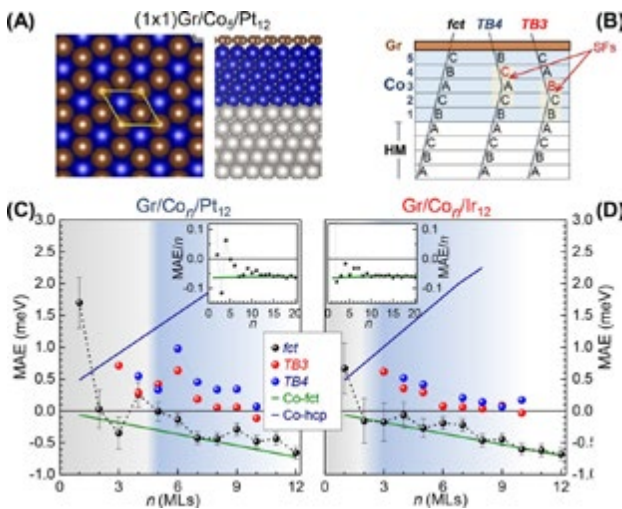


Figure: Calculated magnetocrystalline anisotropy energy (MAE) for $(1 \times 1)\text{-Gr/Co}_n/\text{HM}_{12}$ heterostructures. (A) Representative top and side views of the model used for the ideal fct structure with $\text{HM} = \text{Pt}$ and $n = 5$ MLs. (B) Scheme of the different layer sequences used, without stacking faults (ideal fct) and with one twin boundary starting at the third (TB3) or fourth (TB4) layer of the Co film. (C) and (D) MAE as a function of the Co thickness n calculated for the stacking sequences indicated in panel B, in the case of $\text{HM} = \text{Pt}$ and Ir , respectively. Symbols correspond to $(1 \times 1)\text{-Gr/Co}_n/\text{HM}_{12}$ heterostructures with different stacking sequences (black, red, and blue are used for ideal fct, TB3 and TB4, respectively), whereas continuous lines refer to bulk Co phases (fct and strained hcp indicated in dark blue and green, respectively). Shaded areas emphasize the predicted PMA Co critical thickness, n_c , for ideal fct films. Insets show the MAEs normalized by the Co thickness, n , for the ideal fct films with n up to 20 MLs, in order to illustrate their convergence toward the bulk Co-fct values indicated by the horizontal green line.

Power discontinuity and shift of the energy onset of a molecular de-bromination reaction induced by hot-electron tunneling

Ana Barragán, Roberto Robles, Nicolás Lorente, and Lucía Vitali.

Nanoscale 13, 15215 (2021)

Understanding the structural and chemical stability of organics under applied electrical bias is fundamental to further progress in (electro)-catalysis and (opto)-electronics. This work addresses the dissociation mechanism of halogen atoms and reports on its sharp dependence on the applied electrical power and molecular density of states.

Regardless of the optical or thermal excitation or field-driven injection of electrons, their interaction with organic structures is critically important for the development of many applications. The immediate, albeit transitory, electron occupation of well-defined molecular orbitals, or the related energy exchange process, is beneficial for the activation of chemical reactions. However, for the same reason, the electron interaction itself constitutes one of the main limits to the structural stability of organics in (opto)-electronics.

This collaborative work between the Donostia International Physics Center (DIPC), the University of the Basque Country (EHU/UPV) and the Material Physics Center (MPC) addresses the mechanism of molecular dissociation under applied bias by injecting electrons in tunneling conditions. Specifically, the researchers have

correlated the energy of debromination of an aryl group with its density of states in a self-assembled dimeric structure of 4'-bromo-4-mercaptobiphenyl adsorbed on an Au(111) surface. The authors have observed that the electron-energy range where the molecule is chemically stable can be extended, shifting the bias threshold for the rupture of the C-Br bond continuously from about 2.4 to 4.4 V by changing the electron current. Correspondingly, the power needed for the dissociation changes; however, surprisingly, it drops sharply to about 20% of the original value at 3.6 V. The abrupt change identifies two different reaction regimes and the contribution of additional molecular resonance states.

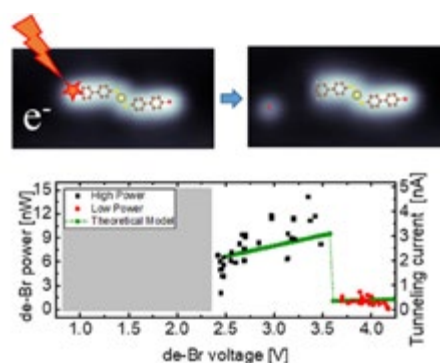


Figure: Graphical representation of the electron induced dissociation of Br atoms in the $\text{Au}(\text{Br-MBP})_2$ complex. The reaction onset can be controlled and shifted for almost 2eV from 2.4eV, however, the reaction power changes sharply when additional molecular resonances are involved.

A molecular transistor controlled through proton transfer

Daniel Weckbecker, Pedro Braña Coto, and Michael Thoss.

Journal of Physical Chemistry Letters 12, 413 (2021)

In this work, the authors have used density functional theory methods and the non-equilibrium Green's function formalism to investigate the possibility of implementing a molecular transistor based on a graphene-molecule junction using a reversible intramolecular proton transfer reaction to control the conductance state of the molecule in the junction.

The ongoing trend in device miniaturization is pushing current semiconductor technologies to their efficiency limit. With the decrease in size, electronic devices are prone to suffer from increasing leakage currents and undesired thermal effects due to high power densities. In search of alternatives to overcome these limitations, the idea of using single molecules to build electronic components has attracted great interest.

In this context, Weckbecker *et al.* have explored the possibility of using a molecule-graphene junction where the molecular bridge features two differently conducting states (ON/OFF) that can be interconverted through a proton transfer process to implement a molecular transistor. For this, they have characterized the ON/OFF switching process, which has been shown to be intrinsic to the molecular bridge and robust with respect to changes of the type of the termination of the graphene leads. Furthermore, the researchers have shown that the ON/OFF state of the molecular bridge can be controlled using an external electrostatic gate field, which enables the possibility of using this molecular junction as a molecular field effect transistor. Finally, they have also verified that the mechanism is robust with respect

to structural changes of the molecular bridge, paving the way for the optimization of the ON/OFF conductance ratio and the gate field strength needed to trigger the intramolecular proton transfer process.

All in all, this work has shown that molecular nanojunctions exhibiting an intramolecular proton transfer mechanism can be used to realize a molecular transistor.

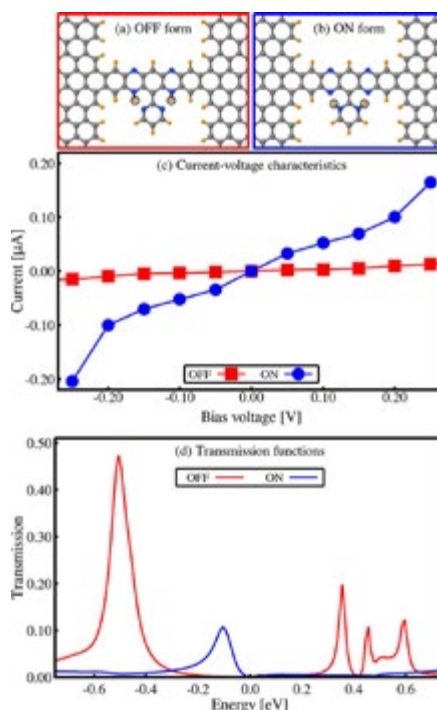


Figure: Molecule-graphene nanojunction investigated in this work with the molecular bridge in the (a) low conductance (OFF) and (b) high conductance (ON) tautomeric, (c) the corresponding current-voltage characteristics and (d) zero-bias transmission functions of the junction in these two forms. The black circles in (a) and (b) indicate the hydrogen atoms involved in the proton transfer process.

Metallic carbon nanotube quantum dots with broken symmetries as a platform for tunable terahertz detection

Gilles Buchs, Magdalena Marganska, John W. González, Kristjan Eimre, Carlo A. Pignedoli, Daniele Passerone, Andres Ayuela, Oliver Gröning, and Dario Bercioux.

Applied Physics Reviews 8, 021406 (2021)

Terahertz (THz) radiation is all around us. For example, this page emits blackbody radiation mainly in the THz region (broadly from 0.3 THz to 30 THz). Because terahertz radiation begins at a wavelength of around one millimeter and proceeds into shorter wavelengths, it is sometimes known as the submillimeter band, and its radiation as submillimeter waves, especially in astronomy.

This band of electromagnetic radiation can be regarded either as microwave radio waves or far-infrared. The technology for its generation and manipulation is in its infancy; that is why engineers talk about the THz gap (in this case, from 0.1 to 10 THz). One of the reasons is that THz radiation from traditional microwave sources is usually too weak to have any measurable impact on the

properties of materials. The situation drastically changed at the beginning of the 2000s, when the technique of optical rectification with phase matching in crystals lacking inversion symmetry such as lithium niobate was developed. This technological breakthrough enabled the development of table-top sources of single-cycle THz pulses with field strengths comparable to the intrinsic field strength in a wide range of strongly correlated materials. Consequently, it became possible to modify their intrinsic fields to engineer new dynamic states of materials.

In condensed matter physics and in general, THz radiation is an efficient tool to investigate a multitude of low-energy excitations existing in the THz region. Important examples are resonances of phonons and plasmons (collective lattice and electron vibrations, respectively), spins, intersubband transitions (subbands are electronic energy bands formed in quantum wells, in which the electrons are confined in two directions), excitons (bound electron-hole pairs), macro-molecular vibrations and molecular rotations.

THz radiation can penetrate most dielectric materials non-invasively, opening the way for numerous possible applications in the fields of medicine, security, chemi-

cal spectroscopy, and data transmission, notably in the framework of the future 6G cellular network. This is why photodetection and emission in the THz regime have recently attracted much attention from fundamental and applied research communities.

The authors have proposed a theoretical scheme for a fully tunable THz detector based on carbon nanotubes. Specifically, using numerical simulations and scanning tunneling spectroscopy, Buch *et al.* show that breaking simultaneously various symmetries in metallic nanotube quantum dots of arbitrary chirality strongly relaxes the selection rules in the electric dipole approximation and removes energy degeneracies. This leads to a rich-

er set of allowed optical transitions spanning frequencies from 1 THz to several tens of THz for a ~10 nm quantum dot. The researcher team proposed a terahertz detector device based on a metallic single-walled carbon nanotube quantum dot defined by artificial defects based on these findings. The operating regimes range from a high-resolution gate-tunable THz sensor to a broadband THz detector, depending on its length and contacts transparency. Their calculations indicate that the device is mainly unaffected by temperatures up to 100 K, making carbon nanotube quantum dots with broken symmetries a promising platform to design tunable terahertz detectors that could operate at liquid nitrogen temperatures.

“The proposed device is largely unaffected by temperatures up to 100 K, making carbon nanotube quantum dots with broken symmetries a promising platform to design tunable THz detectors that could operate at liquid nitrogen temperatures.”

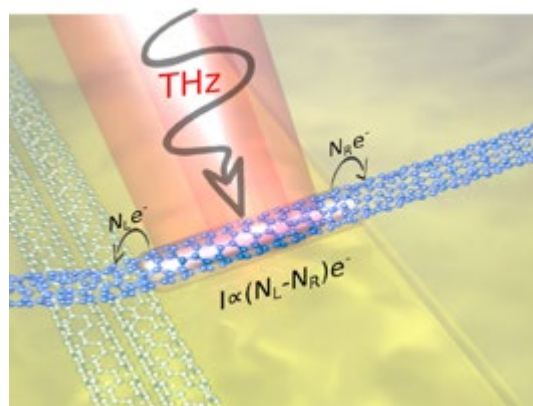


Figure: Proposed device to be used as either a high-resolution gate-tunable terahertz sensor or a broadband terahertz detector.

Simple accurate predictor for conventional superconductivity

Francesco Belli, Trinidad Novoa, J. Contreras-García, and Ion Errea

Nature Communications 12, 5381 (2021)

Through the analysis of a large set of hydrogen based superconductors, the authors identify that a large degree of electronic localization in the interstitial sites is key to enhance their critical temperature. Such localization is measured through a newly defined magnitude, named “networking value”. This quantity is able to predict, with reasonable accuracy, the superconducting critical temperature in conventional hydrogen based superconductors.

The recent discovery of room temperature superconductivity has proven the outstanding potential of hydrogen rich systems. If this class of compounds could be engineered for applications to our daily world, their extraordinary features would introduce a technological revolution through lossless electrical transport and ultra efficient electrical engines or generators. For this reason, an intense joint theoretical and experimental effort is being developed currently to expand the practical usability of hydrogen based superconductors. In this effort, theory has a prominent role in guiding experiments forward by proposing possible stable compounds and by establishing the key ingredients that lead to superconductivity.

This theoretical work investigates a large set of hydrogen based materials predicted to be superconductors, attempting to highlight the specific general features giv-

ing rise to high critical temperatures. From the obtained results, it appears clear that the appearance of an ordered network of covalent bonds is able to boost the superconducting properties. Furthermore, the group then continues by identifying a magnitude called “networking value” related to the ability of the material to create crystal sized networks based on electronic localization features at the interstitial sites (Figure). This quantity is able to predict, with reasonable accuracy, the critical temperature of hydrogen based superconductors better than any other descriptor analyzed so far.

The identification of the networking value opens the possibility for a fast screening of theoretical predictions, while providing a clear understanding of the structural, electronic and bonding features that enhance conventional superconductivity. Furthermore, it provides a first step towards real space interpretations of conventional superconductivity.

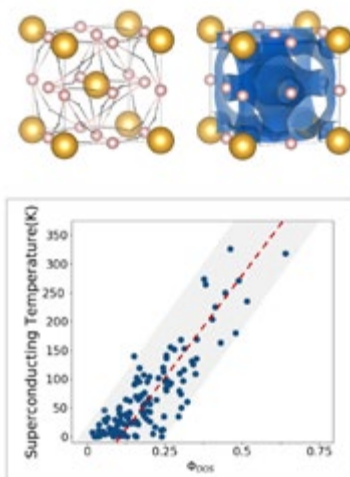


Figure: Example of bonding network and networking value in function of the superconducting critical temperature.

Coexistence of superconductivity and interfacial exchange

Alberto Hijano, Stefan Ilić, Mikel Rouco, Carmen González-Orellana, Maxim Ilyn, Celia Rogero, P. Virtanen, T. T. Heikkilä, S. Khorshidian, M. Spies, N. Ligato, F. Giazotto, E. Strambini, and F. Sebastián Bergeret.

Physical Review Research 3, 023131 (2021)

The Mesoscopic Physics group, in a close collaboration with experimental colleagues, developed the theory to describe the coexistence of superconductivity and an exchange field generated at the interface between a magnetic insulator and a superconducting thin film. On the one hand, these results demonstrate the important role of the superconductor layer thickness, which is particularly relevant for the fabrication of high-quality samples suitable for applications. On the other hand, the agreement between theory and experiment demonstrates the accuracy of the present theory, which, originally developed for homogeneous situations, is now generalized to highly inhomogeneous systems.

Ferromagnetic insulators (FI) can induce an exchange field in an adjacent superconductor (S) via the magnetic proximity effect, which is due to the interfacial exchange interaction between the localized magnetic

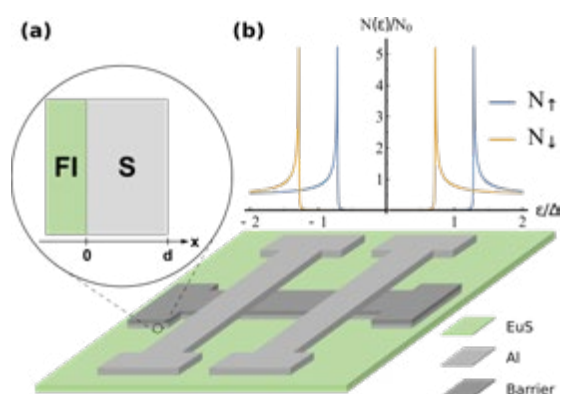


Figure 1: (a) Typical experimental setup and schematic view of the FI/S bilayer. (b) DoS of a homogeneous spin-split superconductor.

moments and the S's conduction band electrons. Such exchange field manifests as a spin splitting. Superconductors with a spin-split density of states (DoS) are proposed for diverse applications, such as topological qubits using Majorana wires, spin valves, thermometry, magnetometers, caloritronic devices, thermoelectricity, and radiation detectors, among others.

A crucial parameter that determines the magnitude of the induced spin splitting in FI/S bilayers is the thickness of the S layer d . In very thin samples, the superconductivity is suppressed by the strong magnetism. By contrast, in very thick samples, the spin splitting is absent at distances away from the interface.

“We have developed a self-consistent microscopic model to optimize the coexistence of superconductivity and the exchange field in devices based on FI/S junctions.”

In this work, the authors calculate the density of states and critical exchange field of FI/S bilayers of arbitrary thickness. From the model presented, Hijano *et al.* determine the range of parameters of interest for applications, where the exchange field and superconductivity coexist.

They show that for $d > 3.0\xi_s$, the paramagnetic phase transition is always of the second order, in contrast to the first-order transition in thinner samples at low temperatures. Here ξ_s is the superconducting coherence length.

Finally, the work compares the author’s theory with the tunneling spectroscopy measurements in several EuS/Al/AlOx/Al samples. If the Al film in contact with the EuS is thinner than a certain critical value, superconductivity is not observed, whereas, in thicker samples, evidence of a first-order phase transition induced by an external field is found. The complete transition is preceded by a regime in which normal and superconducting regions coexist. The group attributes this mixed phase to inhomogeneities of the Al film thickness and the presence of superparamagnetic grains at the EuS/Al interface with different switching fields. The step-like evolution of the tunnel-barrier magnetoresistance supports this assumption.

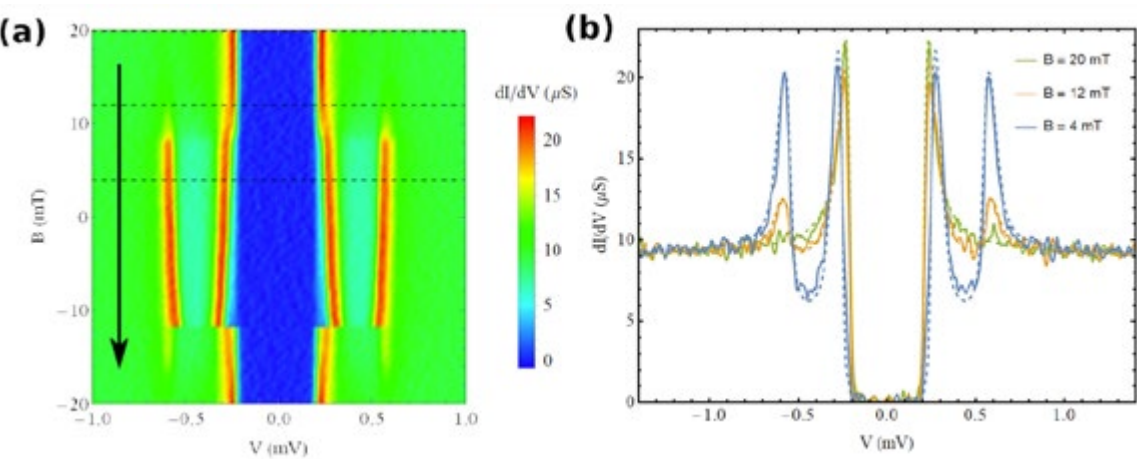


Figure 2: (a) The differential conductance of the FI/S/I/ junction at 30 mK as a function of the external magnetic field and the voltage drop across the junction. The arrow indicates the direction of the magnetic field sweep. (b) dI/dV curves at three different values of B ($B = 4$, $B = 12$ and $B = 20$ mT), indicated by dashed lines in (a). The solid lines correspond to the experimental data, whereas the dashed lines to the theoretical calculation.

Mirror Chern numbers in the hybrid Wannier representation

Tomáš Rauch, Thomas Olsen, David Vanderbilt, and Ivo Souza.

Physical Review B 103, 195103 (2021)

Electron in crystals are usually described in terms of extended Bloch states. An alternative representation is in terms of localized Wannier orbitals. Here, Rauch *et al.* use an intermediate “hybrid Wannier representation”, where states are localized in one spatial direction and extended in the other directions, to study topological properties.

The topology of electronic states in band insulators with mirror symmetry can be classified in two different ways. One is in terms of the **mirror Chern number**, an integer that counts the number of protected Dirac cones in the Brillouin zone of high-symmetry surfaces. The other is via a Z_2 index that distinguishes between systems that have a nonzero quantized orbital magne-

toelectric coupling (“axion-odd”) and those that do not (“axion-even”); this classification can also be induced by other symmetries in the magnetic point group, including time reversal and inversion. A systematic characterization of the axion Z_2 topology has previously been obtained by representing the valence states in terms of hybrid Wannier functions localized along one chosen crystallographic direction and inspecting the associated Wannier band structure.

Here, the researchers focus on mirror symmetry, and extend that characterization to the mirror Chern number. The authors choose the direction orthogonal to the mirror plane as the Wannierization direction and show that the mirror Chern number can be determined from the winding numbers of the touching points between Wannier bands on mirror-invariant planes and from the Chern numbers of flat bands pinned to those planes. In this representation, the relation between the mirror Chern number and the axion Z_2 index is readily established. The formalism is illustrated by means of *ab initio* calculations for SnTe in the monolayer and bulk forms, complemented by tight-binding calculations for a toy model.

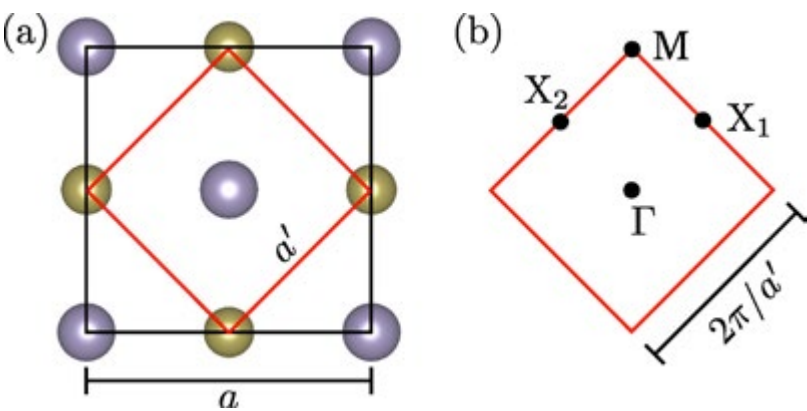


Figure 1: (a) Atomic structure of monolayer SnTe. The black square is the conventional unit cell with lattice constant a , and the red square is the primitive cell with lattice constant $a' = a/\sqrt{2}$. (b) Brillouin zone and high-symmetry points.

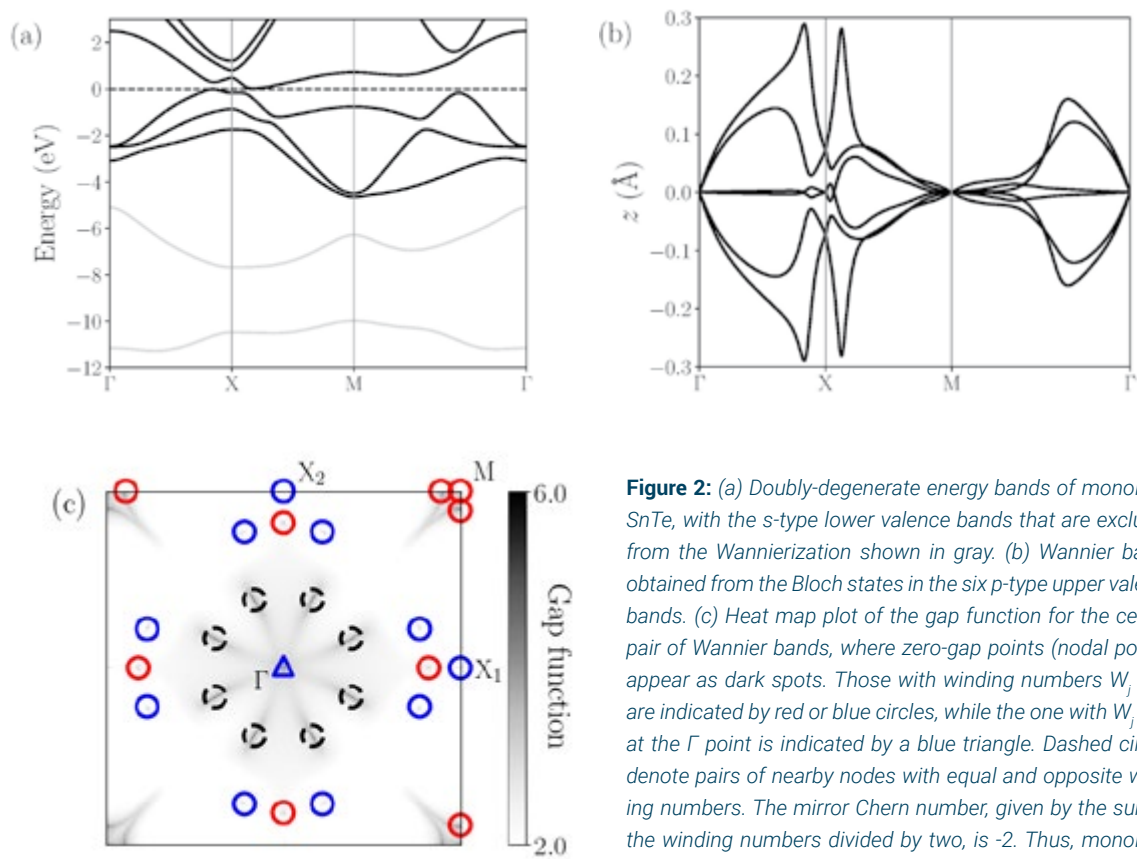


Figure 2: (a) Doubly-degenerate energy bands of monolayer SnTe, with the s-type lower valence bands that are excluded from the Wannierization shown in gray. (b) Wannier bands obtained from the Bloch states in the six p-type upper valence bands. (c) Heat map plot of the gap function for the central pair of Wannier bands, where zero-gap points (nodal points) appear as dark spots. Those with winding numbers $W_j = \pm 1$ are indicated by red or blue circles, while the one with $W_j = -3$ at the Γ point is indicated by a blue triangle. Dashed circles denote pairs of nearby nodes with equal and opposite winding numbers. The mirror Chern number, given by the sum of the winding numbers divided by two, is -2. Thus, monolayer SnTe is a topological crystalline insulator.

A dissolution model of alite coupling surface topography and ions transport under different hydrodynamics conditions at microscale

Jiayi Chen, Pablo Martin, Zhiyuan Xu, Hegoi Manzano, Jorge S. Dolado, and Guang Ye.

Cement and Concrete Research 142, 106377 (2021)

A cement is any of various substances used for bonding or setting to a hard material. A popular one, Portland cement, is a mixture of calcium silicates and aluminates made by heating limestone (CaCO_3) with clay (that contains aluminosilicates) in a kiln. The product is then ground to a fine powder. When Portland cement is mixed with water, it sets in a few hours and then hardens over a longer period of time due to the formation of hydrated aluminates and silicates.

Portland cement contains four main components: alite, belite, calcium aluminate and calcium aluminoferrite. Alite (tricalcium silicate) is the major and characteristic mineral phase. The thermodynamics and kinetics of alite hydration has been studied for more than 100 years and still it is not completely understood.

In the past decades, many hydration models were proposed for the hydration process of Portland cement. These models favored either particle reaction kinetics or integrated reaction kinetics, and focused on the dissolution of cement grains, but individual chemical components were not considered explicitly.

Some models have been proposed in order to predict the dissolution of alite. Some take the vector approach, with arbitrarily chosen hydration kinetics to calculate the hydration rate and convert the amount of hydration product into a volumetric term; however, thermodynamics and ions transport are not taken into account. Others proposed an analytical model to simulate the dissolution of alite. These models described the etch pit formation on the surface of alite, and calculated the corresponding dissolution rate, but diffusion and chemistry were not considered.

In 2019, Pablo Martin, Hegoi Manzano and Jorge S. Dolado proposed a Kinetic Monte Carlo model (KMC) at the nanoscale, which could simulate the dissolution of crystals not only in dilute solutions but also at close-to-saturated conditions. It simulated all dissolution mechanisms at nano/micro scales. Now, an integrated model is proposed to simulate the dissolution of alite under different hydrodynamic conditions at microscale, combining KMC with the Lattice Boltzmann Method (LBM) and the concept of Diffusion Boundary Layer (DBL).

All aspects of the dissolution process are incorporated in the new model. The dissolution of alite itself is modelled with KMC; two multiple-relaxation-time LBM models are used, one to simulate the flow and the other for the transport of ions. The solid-liquid interface is considered using an adapted DBL to calculate the concentration gradient and the dissolution flux. The model is validated with experimental data from literature.

The simulation results show good agreement with published results. At higher initial concentration, the simulation shows a greater dissolution rate than the experimental data. The plateau value is reached at saturated condition, which indicates that the simulation model can be used to predict the dissolution rate of alite under extreme hydrodynamic conditions, i.e., high flow rates.

For a complete study on the dissolution of cement particle, it is necessary to involve all of its components individually and simultaneously. This new model for alite provides a good start point for the simulation of the other cement components.

“An integrated dissolution model is proposed to deal with different hydrodynamics conditions, coupling surface topography and ions transport.”

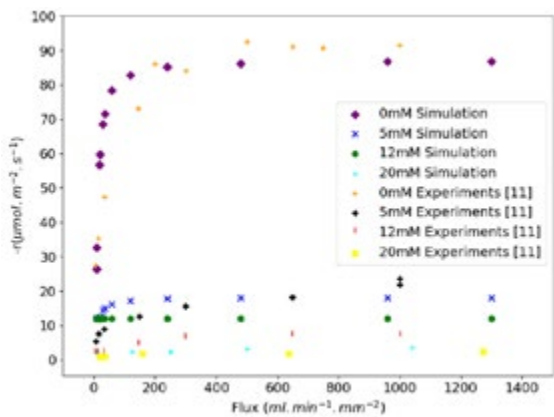


Figure: Influence of the flow rate on the dissolution rate of alite for solutions having different initial calcium hydroxide concentrations. Comparison between the model and available experiments.

Electronic exciton–plasmon coupling in a nanocavity beyond the electromagnetic interaction picture

Antton Babaze, Ruben Esteban, Andrei G. Borisov, and Javier Aizpurua.

Nano Letters 21, 19, 8466 (2021)

A quantum many-body description of the interaction between an exciton and plasmonic resonances in a metallic nanocavity indicates that electronic coupling, often ignored by classical electromagnetic calculations, can strongly modify the optical response of the hybrid system, thus influencing the performance of nanoscale optoelectronic devices.

Plasmonic resonances in metallic nanocavities exploit the collective oscillations of free electrons in metals to confine light into nanometer-sized regions, well below the diffraction limit. This large confinement enables a very efficient excitation and interaction with excitons in molecules, quantum dots and other quantum emitters, as typically described within classical electromagnetic frameworks.

A particularly attractive configuration to optically excite an exciton consists in locating a quantum emitter in

the gap formed between two metallic nanostructures (sketch in top-left panel). When decreasing the separation distance between the particles the confinement of the electromagnetic fields in the gap is enhanced dramatically. In this work, researchers of CFM, in collaboration with Andrei G. Borisov from the Institut des Sciences Moléculaires d'Orsay in France, go beyond the classical electromagnetic description to show that charge-transfer electronic processes can strongly influence the optical response of this type of hybrid plasmon-exciton systems at very short separation distances, of the order of a nanometer, as revealed by quantum many-body calculations based on Time-Dependent Density Functional Theory (TDDFT).

“Electronic quenching of excitons can modify the optoelectronic response of quantum emitters coupled to plasmonic nanocavities.”

The TDDFT calculations demonstrate that the electronic states of the quantum emitter can hybridize with those of the metallic nanocavity (bottom left panel), which leads to a quenching of the exciton and to a weaker optical interaction with the plasmonic resonances, as manifested in clear changes on the strength and energy of the peaks of the absorption spectrum (right panel). For instance, if the exciton is resonant with a plasmonic resonance, the electronic quenching limits the value of the vacuum Rabi splitting that separates energetically the hybrid polaritonic modes that arise when the system is

in the strong coupling regime. The origin of the predicted effects is corroborated by comparing the quantum TDDFT calculations with classical and semi-classical results. Furthermore, the quantum emitter also facilitates the transfer of electric charge between the metallic nanostructures forming the nanocavity, resulting in the emergence of additional low-energy plasmonic modes. Understanding the interplay between the optical and electronic coupling of excitons and plasmonic resonances is important to optimize light sources and to engineer novel optoelectronic devices.

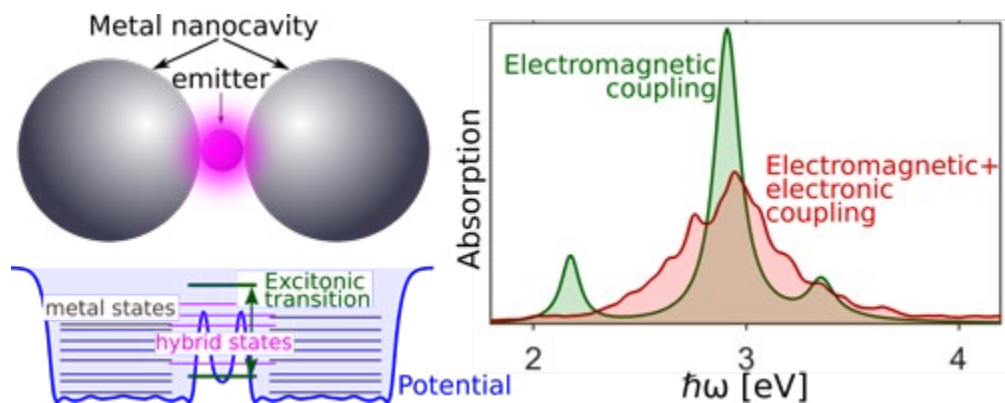


Figure: Electromagnetic and electronic coupling of an emitter and a metallic nanocavity. (Top Left) Sketch of the system considered. (Bottom Left) The electronic coupling between an exciton of the quantum emitter and the metal states of the plasmonic nanocavity results in the emergence of hybrid states that quench the excitonic transition. (Right) Absorption spectra obtained with classical calculations that only consider the electromagnetic coupling (green) or with TDDFT calculations that include both the electromagnetic and the electronic coupling (red). The difference between the TDDFT and classical spectra is mainly due to electronic coupling.

Strong increase in the effective two-photon absorption cross-section of excitons in quantum dots due to the nonlinear interaction with localized plasmons in gold nanorods

Victor Krivenkov, Pavel Samokhvalov, Ana Sánchez-Iglesias, Marek Grzelczak, Igor Nabiev, and Yury Rakovich.

Nanoscale 13, 4614 (2021)

Semiconductor Quantum Dots (QDs) feature high two-photon absorption capability, enabling applications in biosensing and nonlinear optoelectronics. Plasmonic nanoparticles may enhance the electromagnetic field on the nanoscale, which increases the applicability of QDs. Here, the researchers directly measured the enhancement of two-photon absorption in QDs near the plasmonic nanoparticles.

Semiconductor Quantum Dots (QDs) are known for their highly efficient two-photon absorption compared to the conventional organic fluorophores. Due to the

very high values of Two-Photon Absorption Cross-Sections (TPACSS), QDs are widely used for two-photon fluorescent bioimaging, where they ensure a uniquely high contrast, as well as for the fabrication of nonlinear optoelectronic devices operating in the up-conversion mode. However, due to the nonlinear nature of the two-photon absorption process, efficient two-photon excitation of photoluminescence of QDs requires very high laser intensities, which limits their applications. There are two possible ways to increase the two-photon excitation of photoluminescence of QDs: by increasing their photoluminescence Quantum Yield (QY) or by further increasing the TPACS. Plasmonic nanoparticles may act as open nanocavities for increasing the QY via the Purcell effect, but this enhancement is strictly limited by the maximum possible QY value of 100%.

In this work, the authors directly investigated the effect of plasmonic nanoparticles on the effective TPACS of excitons in QDs. They have found that effective TPACS of excitons in a QD-PMMA thin film can be increased

by a factor of up to 12 near the linearly excited gold nanorods. Using gold nanospheres, in which plasmons cannot be excited in the infrared range, as a control system, the researchers have shown that, although both gold nanospheres and gold nanorods increase the recombination rate of excitons, the TPACS is increased only in the case of gold nanorods. They believe that the observed effect of TPACS enhancement is a result of the nonlinear two-quantum energy transfer from the plasmons in gold nanorods to excitons in QDs, which they have supported by numerical simulations. Thus, Krivenkov et al. have developed an approach for directly increasing the effective TPACS of the excitons in QDs by inducing a nonlinear near-field interaction between absorptive exciton transitions in QDs and plasmon modes in plasmonic nanoparticles. The results of this study are expected to expand the applications of two-photon excitation of plasmon–exciton hybrid structures in multi-photon sensing and bioimaging, photodynamic therapy, and fabrication of nonlinear optical photodetectors.

“Here, Krivenkov et al. have specially studied the TPACS of excitons in thin-film hybrid structures based on QDs and gold PNPs and have found effective enhancement of TPACS by a factor of up to 12.”

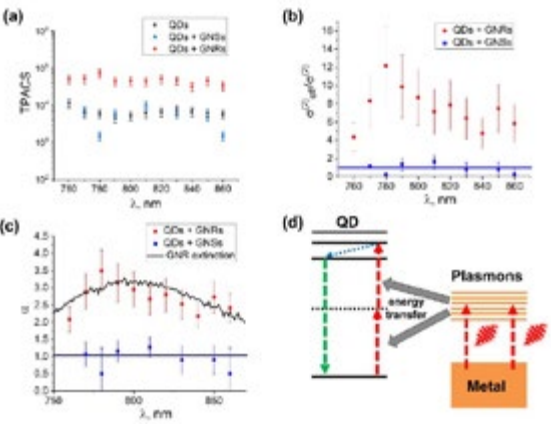


Figure: Effect of gold nanorods on the Two-Photon Absorption Cross-Sections (TPACS) of excitons in semiconductor Quantum Dots (QDs). (a) The measured TPACS of excitons in QDs in the absence of plasmon nanoparticles (black squares), QDs near gold nanospheres (blue triangles), and QDs near gold nanorods (red circles). (b) The calculated change in the effective TPACS of excitons near gold nanorods (red circles) or gold nanospheres (blue squares). (c) The calculated increase in the near-field intensity of plasmon modes in plasmon nanoparticles compared to the intensity of far-field (gold nanorods, red circles; gold nanospheres, blue squares); for comparison, the experimental gold nanorods extinction spectrum (black line) is also shown. (d) The scheme of the plasmon–exciton interaction under external excitation.

Nd³⁺-doped- SiO₂-KLaF₄ oxyfluoride glass-ceramics prepared by sol-gel

María Eugenia Cruz, Jing Li, Giulio Gorni, Alicia Durán, Glenn C. Mather, Rolindes Balda, Joaquín Fernández, and Yolanda Castro.

Journal of Luminescence 235, 118035 (2021)

Neodymium doped SiO₂-KLaF₄ oxyfluoride Glass-Ceramics (GCs) containing 10 and 20 mol % of KLaF₄ NanoCrystals (NCs) were prepared for the first time by sol-gel. Site-selective emission and excitation spectra confirmed the incorporation of Nd³⁺ ions in α-KLaF₄ and β-KLaF₄ crystalline phases with emission of Nd³⁺ most predominant in the β-KLaF₄ NCs.

In the last few decades the growing interest in GCs has revealed the potential of this new class of optical materials, the properties of which, especially the optical ones, significantly improved with controlled crystallization of certain crystalline phases. In the particular case of KLaF₄ nanocrystals, the phonon energy was found to be 262 cm⁻¹, much lower than most fluorides, making it of interest as an efficient host matrix for green, red, and blue up-conversion emission through appropriate doping. Although successful processing of KLaF₄-GCs by Melt-Quenching (MQ) has been reported, preparation by the sol-gel route has not. The sol-gel method offers the possibility of obtaining GCs using a cheap, flexible, and melt-free synthesis route with the possibility of processing as bulk, thin film, and powder materials. Sol-gel

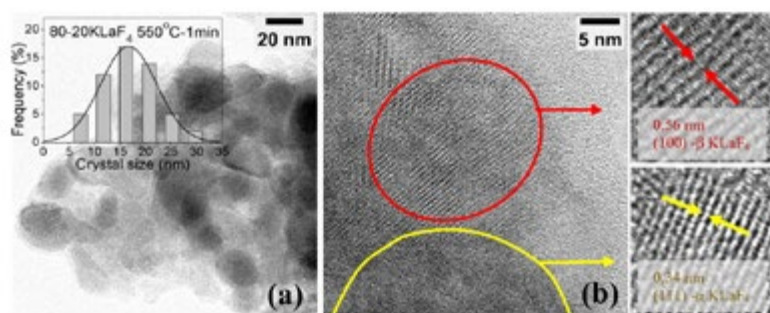


Figure 1: (a) HR-TEM image of 80SiO₂-20KLaF₄ sample treated at 550°C for 1 min with the crystal size distribution. (b) Details of the α and β nanocrystals with their corresponding plane distance.

also allows the final crystal fraction to be controlled by avoiding fluorine loss, which occurs at high temperature during MQ, and thus optical efficiency may be improved.

In this collaborative work carried out by the groups led by Alicia Durán (ICV-CSIC) and Rolindes Balda (CFM, UPV/EHU), transparent $\text{SiO}_2\text{-KLaF}_4$ GCs were, for the first time, successfully obtained by the sol-gel process after heat treatments for just 1 min. Cubic (α -phase) and hexagonal (β -phase) KLaF_4 phases appeared for all heat-treatments, with increasing temperature favoring the cubic-to-hexagonal phase transformation. HR-TEM images confirmed the coexistence of cubic and hexagonal phases with similar nanocrystal sizes to those

estimated by XRD. The spectral features of the emission and excitation spectra together with the lifetimes obtained in the GC sample by using site-selective laser spectroscopy in the $^4\text{I}_{9/2} \rightarrow ^4\text{F}_{5/2}$ transition confirm the incorporation of Nd^{3+} ions in both crystalline phases. The predominant emission of Nd^{3+} ions corresponds to the $\beta\text{-KLaF}_4$ hexagonal phase. The optical behavior differs from that obtained in GC samples prepared by MQ, where the less efficient cubic phase was predominant. It may be concluded, therefore, that the sol-gel method favors the growth of the hexagonal KLaF_4 β -phase, which in general has a higher quantum yield than the cubic polymorph, and is thus a very promising synthesis route for different photonic applications.

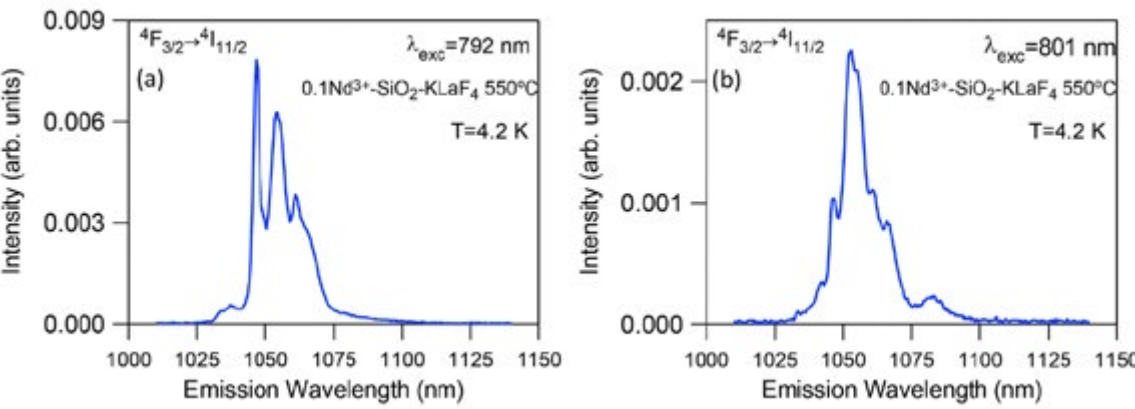


Figure 2: Low temperature emission spectra obtained under excitation at (a) 1046 nm (β phase) and (b) 1055 nm (α phase) for the GC sample.

Self-reporting of folding and aggregation by orthogonal luminophores within a single polymer chain

Julen de La Cuesta, Ester Verde Sesto, Arantxa Arbe, and José A. Pomposo

Angewante Chemie International Edition 60, 3534 (2021)

The folding of some polypeptides, especially enzymes, into perfectly defined three-dimensional (3D) architectures is critical to their function. The specific spatial arrangement of residues ultimately dictates function in 3D-structured proteins. Protein misfolding and aggregation are involved in the onset of many neurodegenerative age-related human disorders. To better understand diseases and design drugs, a variety of methods have been developed to investigate protein folding and to monitor the self-assembly of defective proteins into pathogenic protein aggregates. Among them, photoluminescence techniques are highly valuable due to their high sensitivity and the possibility to select, synthesize and optimize a diversity of photoluminescence probes (luminophores). These compounds allow visualizing protein folding, misfolding and aggregation in vitro and in living cells.

Trying to mimic the outstanding functionalities of proteins, the research field of folding functionalized synthetic polymers to Single-Chain NanoParticles (SCNPs) has flourished in recent years. The folded conformations of SCNPs produce robust nano-objects when

stabilized by covalent bonds as surrogates of disulfide bonds in proteins. Conversely, dynamic SCNPs are obtained by folding of discrete, individual chains arising via noncovalent interactions. Current single-chain technology still lacks nature's exquisite degree of control to generate sophisticated 3D-nanoentities. Nevertheless, some SCNPs do already mimic the outstanding properties of certain antimicrobial polypeptides as well as both the size and function of some metalloenzymes, Intrinsically Disordered Proteins (IDPs), and structural proteins.

However, as observed in the case of defective proteins, some SCNPs systems are not free from multi-SCNPs' aggregation phenomena –arising during synthesis or after long-term storage through inter-chain reactions– that negatively affect their performance, e.g., in catalysis, drug delivery and sensing applications. A visual, self-reporting method to distinguish between individual SCNPs and unbidden multi-SCNPs assemblies with the naked eye, and in the former case the degree of single-chain compaction, would be invaluable in further advancing this field of bioinspired research.

This work reports on a simple and efficient platform to identify both single-chain compaction and inter-molecular aggregation phenomena via photoluminescence based on simultaneous synthesis through Hantzsch ester formation of orthogonal luminophores within the same polymer chain (Figure, panel a). Hence, starting from non-luminescent β -ketoester-decorated chains, intra-molecular compaction is visually detected through fluorescence arising from Hantzsch fluorophores generated as intra-chain connectors during folding (Figure, panel b). Complementary, inter-molecular association is identified via Aggregation-Induced Emission (AIE) from orthogonal luminophores displaying intense photoluminescence at redshifted wavelengths after formation of multi-SCNPs assemblies (Figure, panel c). The method, which is simple and highly accurate, holds promise to perceive at a glance the presence / absence of detrimental multi-chain aggregates affecting the performance of SCNPs in catalysis, sensing, recognition, and so on.

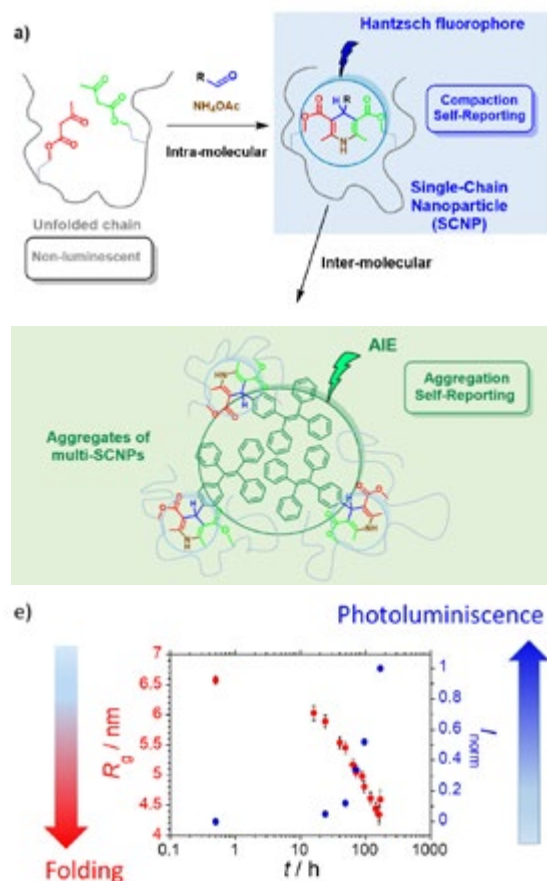


Figure: (a) Strategy for the synthesis of orthogonal luminophores based on Hantzsch ester formation within a β -ketoester-decorated chain for self-reporting of intra-molecular compaction (folding) and inter-molecular association (aggregation). (b) Inverse relationship between single-chain size reduction, as determined by in situ SAXS kinetic measurements and photoluminescence emission observed during single-chain folding. (c) Photographs showing inter-molecular association of SCNPs in solvent (THF) / non-solvent (EtOH) mixtures at different volume ratios under 365 nm UV illumination upon increasing EtOH concentration.

Reaching the ideal glass in polymer spheres: Thermodynamics and vibrational density of states

Xavier Monnier, Juan Colmenero, Marcel Wolf, and Daniele Cangialosi.

Physical Review Letters 126, 118004 (2021)

Glasses, though in the solid state, differ from crystals as they exhibit no long-range order in the atomic distribution. In general, a liquid of any kind can be cooled down below its melting temperature, provided that large cooling rates are used to avoid crystallization. Further cooling leads to the formation of a glass – at a temperature addressed as glass transition temperature, T_g – whose thermodynamic state profoundly depends on its thermal history. Once in the glassy state, spontaneous evolution towards low energy states, known as physical aging, takes place.

A deep unresolved question in glass science regards the equality of the glass entropy with that of the crystal at

a finite temperature, addressed as the Kauzmann temperature, T_k , implying an entropy catastrophe with the paradoxical scenario of a liquid having smaller entropy than that of the crystal at $T < T_k$. To avoid this unpalatable scenario, it has been largely debated whether a true second order thermodynamic transition, the “ideal” glass transition, at T_k takes place. An important aspect related is that, apart from the thermodynamic view, the achievement of low energy glasses may deeply affect the glass Vibrational Density Of State (VDOS). An excess in the VDOS, addressed as the boson peak, is observed in glasses whose magnitude decreases with the energy.

Accessing low energies in bulk glasses is unfeasible due to the astronomical time scales required. Indeed, the transformation of the supercooled liquid into a glass takes place at large energies and subsequent glass equilibration below T_g is extremely slow. Hence, the authors exploited the ability of glasses with large free interfaces to access low energy states. Specifically, aggregates of spheres of a polymeric glass former were aged well below their T_g and characterized by calorimetry and inelastic neutron scattering to monitor the thermodynamic state and the VDOS, respectively.

The results show that, when aged at appropriate temperatures, glassy spheres attain a thermodynamic state corresponding to an ideal glass in about one day, indicating

that increasing glasses' free interface induces a tremendous reduction of the timescale to recover equilibrium. Via a relaxation process with finite timescale deep in the glassy state, this acceleration allows attaining glass energies relevant to detect a kink in the enthalpy, identified with the transformation from the standard into the ideal glass (see Figure, upper right panel). In the ideal glassy state, the boson peak disappears (see Figure, lower right panel), thus rendering the VDOS alike that of crystals.

“The existence of the ideal glass is proved by aging glasses with a large amount of free interfaces. The boson peak in the ideal glass is suppressed.”

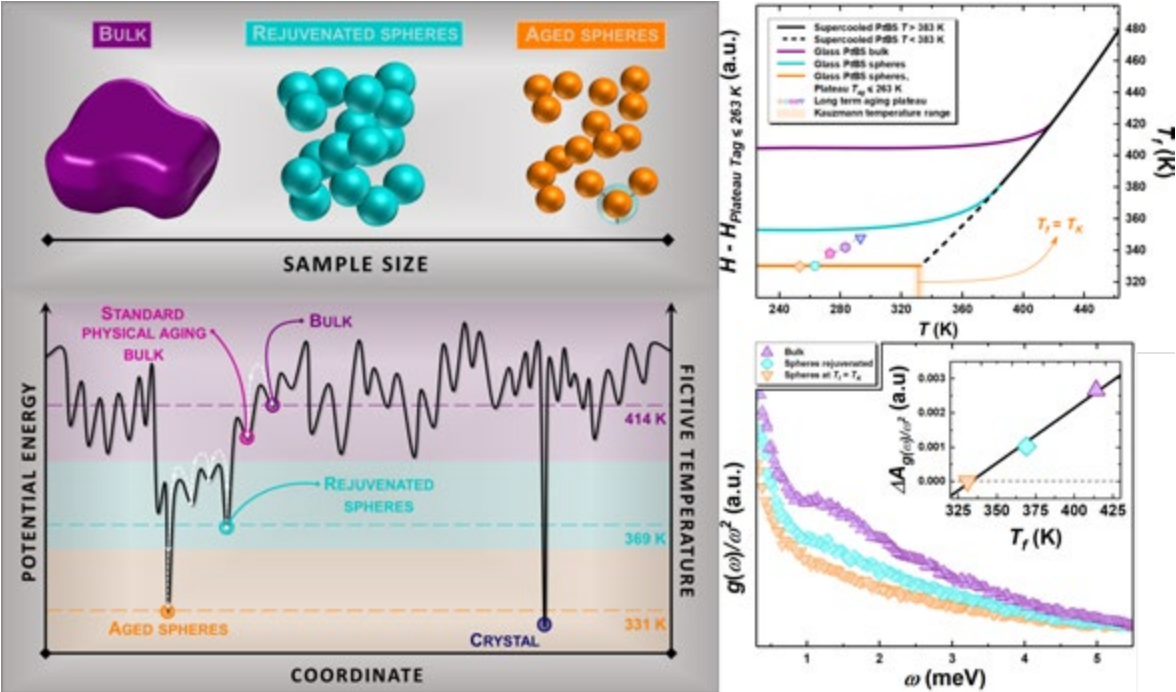


Figure: (Left panel) Schematic representation of the potential energy landscape for bulk and sphere glasses, showing how deep in the landscape the latter system can fall. (Right upper panel) Thermodynamic plot showing the glass enthalpy of bulk and polymer spheres, the equilibrium (supercooled) line and the kink in the enthalpy at the ideal glass transformation. (Right lower panel) Reduced VDOS for bulk and polymer spheres before aging (rejuvenated) and in the ideal glass state. The inset shows the relation between the glass thermodynamic state and the VDOS.

Reconfigurable artificial microswimmers with internal feedback

Laura Alvarez, Miguel-Angel Fernandez-Rodriguez, Angel Alegria, Silvia Arrese-Igor, Kai Zhao, Martin Kroger, and Lucio Isa.

Nature Communication 12 (2021) 4762

Self-propelling microparticles are often proposed as synthetic models for biological microswimmers with internal feedback. Here, this research team presents an experimental realization of reconfigurable active colloids. In particular, Álvarez et al connect the propulsion of the active colloidal clusters to their temperature-dependent size and dielectric properties, mediated by the presence of soft, thermo-responsive microgels, which the authors extensively characterize.

The ubiquity and success of motile bacteria are strongly coupled to their ability to autonomously adapt to different environments. Realizing artificial microswimmers with similar adaptation capabilities might substantially impact technologies ranging from

optimal transport to sensing and microrobotics. Existing approaches at the colloidal scale mostly rely on external feedback. On the contrary, endowing artificial microswimmers with an internal feedback mechanism remains an elusive task.

A promising route to achieve this goal is to exploit the coupling between particle shape and motility. Here, an approach to fabricate reconfigurable microswimmers is presented, relying on a simple combination of standard "hard" particles and soft responsive colloids using asymmetric colloidal clusters (dumbbells) containing both PolyStyrene (PS) microparticles and soft thermo-responsive microgels. The PS particles convert an external light intensity signal into heat, causing the transition of the attached microgel from a swollen to a collapsed state, which can be reversed by reducing the illumination. When the microgel reconfiguration is coupled to self-propulsion, the result is a reconfigurable microswimmer with internal feedback triggered by the sensing of a light stimulus orthogonal to its propulsion scheme.

Upon applying an AC voltage at a frequency $f = 1$ kHz to an aqueous suspension, the dumbbells self-propel with velocities around $3\text{--}6\text{ }\mu\text{m s}^{-1}$. We tracked the motion of

the dumbbell particles under epifluorescence illumination encoding the input signal for particle reconfiguration. A systematic quantification shows that the velocity changes caused by illumination are fully reversible with response times of a few seconds. To rationalize the results, the team evaluated the Clausius–Mossotti factor connecting the velocities with the solvent viscosity, the particle radius, and dielectric properties. For doing so, they used dielectric spectroscopy to extract the permittivity ϵ'_p and conductivity σ'_p of a single microgel (see Figure 1) from the direct measurements of the corre-

sponding effective values of a microgel suspension as a function of frequency and temperature.

The obtained results (see Figure 2) demonstrate that programmable adaptive behavior can be implemented by exploiting soft responsive colloids as components of artificial microswimmers. The selection of microgels with given properties (e.g., size, swelling ratio, and dielectric properties) will render active clusters which spontaneously respond to temperature changes in a programmed fashion.

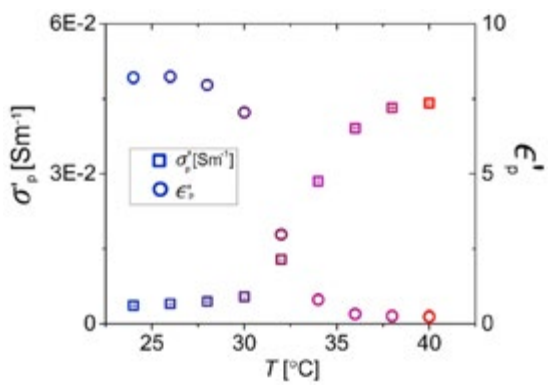


Figure 1: Permittivity (ϵ'_p , open circles) and conductivity (σ'_p , open squares) vs. T at $f = 1$ kHz obtained from the dielectric measurements of a microgel suspension as a function of frequency and temperature.

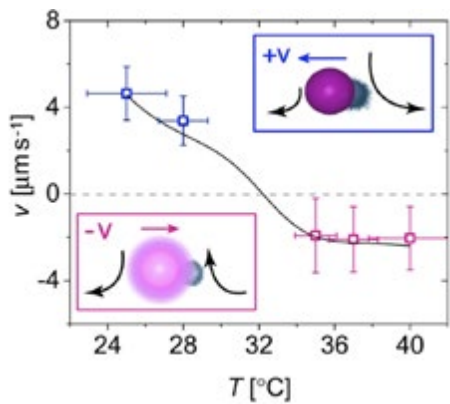


Figure 2: Experimental values (symbols) and theoretical prediction (solid line) of dumbbells' velocity as a function of temperature. The inset schemes indicate the flows and final propulsion direction.

Emergence of dynamical disorder and phase metastability in carbon nanobowls

Mattia Gaboardi, Ian Silverwood, Balthasar Braunewell, Jay Siegel, and Félix Fernández-Alonso.

Carbon 183, 196 (2021)

The curved “nanobowl” corannulene is a fascinating molecule, topologically corresponding to one-third of the celebrated Buckminsterfullerene C60. Emerging applications of this seemingly simple molecular system in its condensed solid and fluid phases include the storage of chemical and thermal energy.

In this particular work, the authors have used radiation-scattering techniques (neutron and synchrotron X-rays) in combination with thermophysical measurements to unveil the microscopic mechanisms underpinning its phase behavior within the solid and liquid phases at ambient pressure. For the first time, Gaboardi et al identify the presence of a well-defined solid-to-solid transition well below the melting point.

Contrary to naïve expectation, detailed analysis of the neutron-spectroscopy data below and above this pre-melting transition signals the emergence of correlated relaxational dynamics in the picosecond domain within both thermodynamically stable solid phases of the material. The researchers also find that these are progressively responsible for the suppression of molecular and supramolecular order over mesoscopic length scales, and are associated with the formation of high-symmetry rotor-like states exhibiting localized stochastic motions. Corannulene is certainly not a canonical solid, but rather exhibits a rich phenomenology linked to this viscoelastic response.

“State-of-the-art radiation-scattering techniques (neutron & synchrotron X-rays) unveil the emergence of dynamical disorder in carbon nanobowls.”

Upon cooling from the melt, a robust hysteresis has also been discovered, associated with the existence of hitherto-unknown metastable liquid (deep-supercooled) and disordered-solid phases. This behavior is markedly different from that observed in the quintessential buckminsterfullerene C₆₀ or other chemically

substituted fullerene adducts studied to date at this level of detail. These results evince new and yet-to-tapped opportunities for the use of the stable and metastable phases of corannulene in novel applications exploiting the emergence of dynamical disorder at the nanoscale.

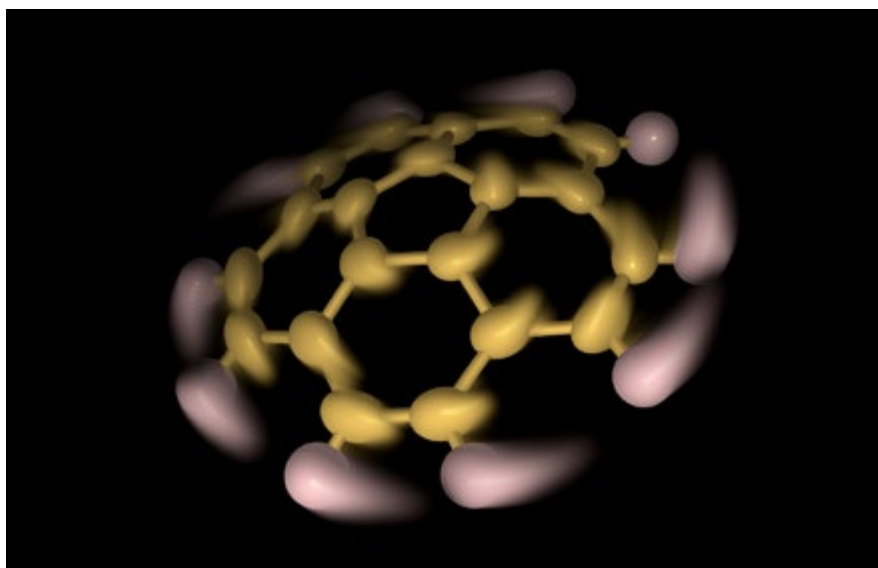


Figure: *Cartoon highlighting the emergence of dynamical disorder in corannulene, well within its low-temperature phase.*



FACILITIES & EXTERNAL SERVICES

CFM infrastructure has been envisioned to characterize nanoscale materials with high sensitivity. Thus, the CFM headquarters was built based on sophisticated architectural and engineering solutions to create a unique environment, free of electromagnetic interference and with an ultralow level of vibration. Since the opening of CFM headquarters in 2010, state-of-the-art facilities have been launched progressively, which complete a set of very sophisticated and specialized experimental techniques, ready to give response to the needs in advanced materials characterization. These needs involve both generic research in nanomaterials, as well as specifically targeted systems of interest in energy and biological environments, perfectly aligned with the Smart Specialization Strategy (RIS3) and the 2030 Science, Technology and Innovation Plan (PCTI 2030) of the Basque Country, as well as with the IKUR Strategic lines defined by the Basque Dep. of Education.

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 Tunnel Microscope, STM). These two techniques can be used either jointly or separately. The ARPES instrument allows achieving ultra-high resolution (0.1 degrees, 5 meV) and can deal with samples at low temperature (40K). Samples can be prepared independently at two different preparation chambers and they can be inserted in the instrument via a fast-entry lock.

SURFACE CHEMICAL-PHYSICS LAB

The “Surface Chemistry” laboratory is equipped with an Ultra High Vacuum chamber combining different surface characterization techniques: X-Ray Photoemission Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), Low Energy Electron Diffraction (LEED) and Scanning Tunnel Microscopy (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 characterization of samples by means of a homemade Magneto Optic Kerr Effect (MOKE, 15-300 K, 0.1 Tesla) and a 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 characterization 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 characterization.

PHOTONICS

LASER SPECTROSCOPY LAB

In the “Laser Spectroscopy” laboratory, continuous and time-resolved (with nano-picoseconds excitation laser sources) spectroscopy systems with high spectral resolution in the ultraviolet-visible-infrared (UV-VIS-IR) radiation domains, together with low temperature facilities (2K), are used to characterize the properties of rare-earth- doped materials for lasing, spectral conversion, energy transfer and laser cooling. A homemade photoacoustic spectrometer is also available. These facilities are physically located at the Engineering School of Bilbao (out of the CFM main premises in Donostia / San Sebastián).

ULTRAFAST SPECTROSCOPY LAB

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

NANOPHOTONICS AND NANOMATERIALS SYNTHESIS LAB

The “Nanomaterials and Spectroscopy” group runs a laboratory for the synthesis of metallic and semiconducting nanoparticles, nanocrystals and nanocomposites, and another one for the characterization of their optical properties. The “Nanomaterials Synthesis Lab” is equipped with a fume hood, benches and state of the art equipment for colloidal synthesis, including a spin coater, centrifuges, thermocycler, thermostats, cryostat, high-precision

programmable syringe and micropumps and balances. The “Nanophotonics” laboratory hosts a scanning confocal time-resolved photoluminescence microscopy setup (MicroTime200) 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 a single nanoparticle/molecule level with a wide range of capabilities: 2D and 3D confocal photoluminescence microscopy imaging, single-molecule imaging, 2D and 3D Fluorescence Lifetime Imaging (FLIM), the minor carrier’s lifetime mapping, carrier’s recombination dynamics, Resonance Energy Transfer (FRET).

Other available set-ups in these two labs include:

- QUEPRO high-performance spectrophotometer connected to IX71 Olympus microscope for micro-photoluminescence spectroscopy
- Two high-resolution UV-Vis-NIR spectrophotometers (Maya2000Pro, Ocean Optics) for real-time spectra acquisition
- 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 a wide range of flow rates

FACILITIES

- 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)
- Equipment for study photothermal effect on plasmonic nanoparticles: four- wavelengths (670, 808, 940, 1064 nm), fiber-coupled diode laser system coupled to a four-window sample holder (Qpod 2e) with internal temperature control. Small-area led Solar Simulator type AAA (Pico, G2V) covering spectra range from 340 to 1500 nm with 30 channels
- A set of laser systems, including continuous wave lasers covering the ultra violet, visible and infrared regions, for producing different photon states: a 633nm, 10mW, He-Ne laser (from Thorlabs); a 403nm, 100mW, diode (from Toptica); a 680nm, 50mW, diode (from Toptica); and an 808nm, 10mW, diode (from Thorlabs)
- A source of entangled photons based on a periodically poled potassium titanyl phosphate (ppKTP) crystal
- Optically addressable cryostat, equipped with state-of-the-art nanopositioners, for cooling down nanostructures and nanoparticles to cryogenic temperatures (attoDRY 100 model from Attocube)
- A set of spatial light modulators (from Cambridge Correlators), polarizers (from Thorlabs and Standa) and Single Photon Counting Modules (SPCM, APDs SPCM-AQ4C model from Excelitas), for analyzing the photons interacting with nanostructures at cryogenic temperatures
- Microwave generators and amplifiers (SMB100A model from Rohde & Schwartz), for addressing the electronic states of Nitrogen Vacancy centers in diamond

MATERIALS SYNTHESIS LAB

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

QUANTUM NANOPHOTONICS LAB

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

- Three optical tables for manipulating the polarization as well as spatial and frequency degrees of freedom of entangled and single photon states: 1200 x 2400 x 305 mm table with isolators (784-655-12DR model from TMC), 1500 x 3000 x 305 mm table with isolators (784-675-12DR model from TMC) and 900 mm x 1800 mm x 305mm table with isolators (from Newport)

POLYMERS AND SOFT MATTER

DIELECTRIC SPECTROSCOPY LAB

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

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

MICROSCOPY LAB

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

- Absolute molecular mass distribution meter: Agilent 1200 GPC-SEC Analysis System + Light scattering Wyatt miniDAWN TREOS, viscosimeter ViscoStar II and Optilab rEX Refractive Index Detector
- Nanoparticle size and z-potential meter: Malvern Zetasizer Nano
- Viscometers: EMS-1000 and Malvern SV-10 Vibro
- Surface tension meter: Contact Angle meter OCA 15 EC DataPhysics Instruments GmbH
- Liquid/solution density meter: ANTON PAAR, DMA 4500 M model
- UV-VIS spectrometer: Agilent 8453A with Peltier thermostated cell holder, T-controller 89090A
- Close vessel microwave assisted reactor: CEM Discover SP System (200-550K, 0-27 bar)

FACILITIES

THERMAL CHARACTERIZATION LAB

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

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

RHEOLOGICAL CHARACTERIZATION LAB

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

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

ABSORPTION SPECTROSCOPY TECHNIQUES LAB

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

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



X-RAY LAB

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

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

LIGHT SCATTERING LAB

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

HIGH PERFORMANCE COMPUTING (HPC) 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 of 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

MPC-CFM offers external services based on the center equipment and infrastructure to academic and industrial users. Thus, external services are measurements and materials' characterization work carried out by MPC-CFM qualified researchers and technicians at MPC-CFM's facilities, for researchers and technologists from different research fields and businesses. The MPC-CFM external services that can be commissioned are as follows:

DIFFERENTIAL THERMAL ANALYSIS (DTA)

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

ISOBARIC THERMAL EXPANSION

The service offers the characterization of polymer and soft matter samples by means of dilatometry and PVT measuring system, using a L75V (100 - 800 K) from Linseis, and a pVT100 (200 - 550 K, 200 - 2500 bar) from Thermo Haake, respectively.

ABSORPTION SPECTROSCOPY IN TERAHERTZ (THZ) DOMAIN

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

DIELECTRIC CHARACTERIZATION

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

SMALL-ANGLE X-RAY DIFFRACTION

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

MATERIALS SURFACE CHARACTERIZATION

The service offers the surface characterization of materials by means of X-ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoemission Spectroscopy (UPS), Atomic Force Microscopy (AFM) and Scanning 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 PERFORMANCE 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

At a glance

82%

Published in the
framework of international
collaborations

Q1 WOS: 59%
Q1 SCOPUS: 86%

H-Index
143

216

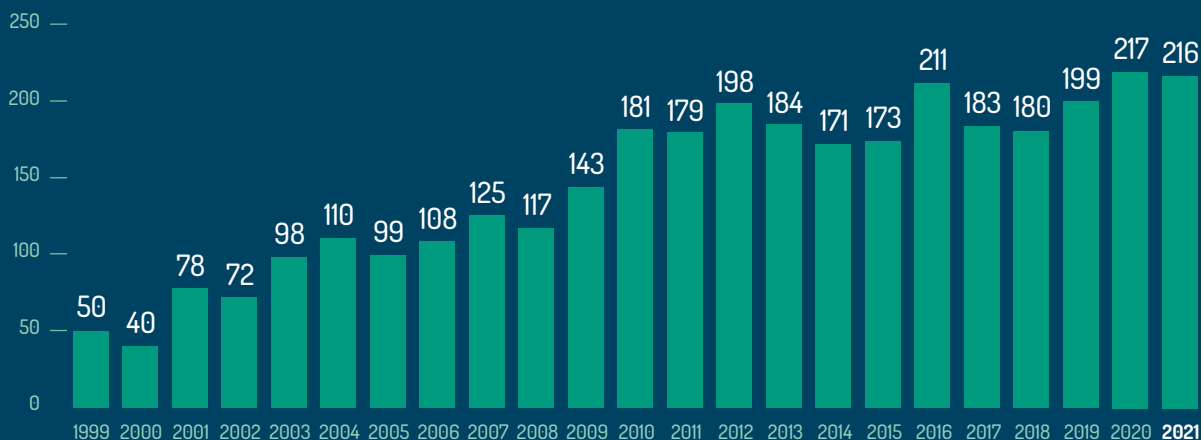
ISI Publications

D1 WOS: 29%
D1 SCOPUS: 41%

ISI Web of Science citations
14 778^{*} in 2021

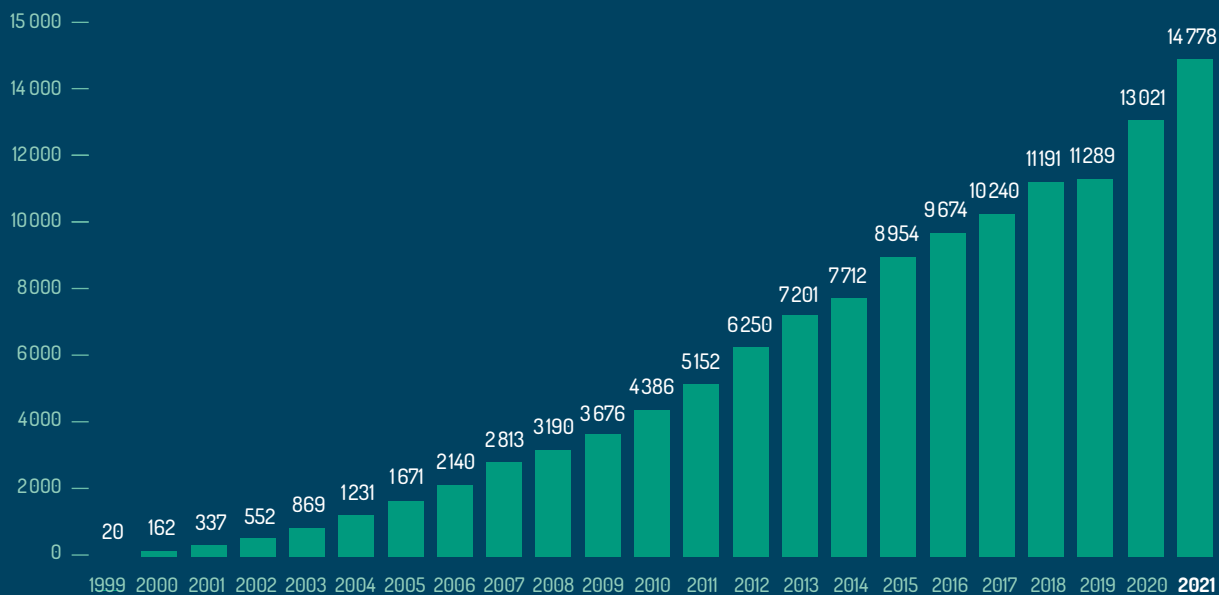
*As of March 2022

PUBLICATIONS



Total number of ISI publications *
since 1999 as of March 2022: **3116**

CITATIONS



Total number of ISI citations since 1999: **132 071**
H index (March 2022): **143**

Total number of top publications*:

65

Journal	Number of articles	Impact factor
Chemical Reviews	1	60.62
Nature	1	49.96
Nature Photonics	1	38.77
Advanced Materials	3	30.85
Nature Physics	2	20.03
Applied Physics Reviews	1	19.16
Advanced Functional Materials	1	18.81
Advanced Science	1	16.81
ACS Nano	5	15.88
Angewandte Chemie- International Edition	5	15.34
Nature Communications	8	14.92
Laser & Photonics Reviews	1	13.14
Nano Letters	8	11.19
Cement and Concrete Research	5	10.99
Chemical Science	1	9.82
Chemistry of Materials	1	9.81
Carbon	2	9.59
Physical Review Letters	7	9.16
Nanophotonics	1	8.45
Nanoscale	8	7.79
ACS Photonics	2	7.53

* With impact factor larger or equal than that of ACS Photonics

PUBLICATIONS

1 Large perpendicular magnetic anisotropy in nanometer-thick epitaxial graphene/Co/heavy metal heterostructures for spin-orbitronics devices

Blanco-Rey M, Perna P, Gudin A, Diez JM, Anadon A, Olleros-Rodriguez P, Costa LD, Valvidares M, Gargiani P, Guedeja-Marron A, Cabero M, Varela M, Garcia-Fernandez C, Otrokov MM, Camarero J, Miranda R, and Arnau A. ACS Applied Nano Materials 4, 4398 (2021)

2 Additive manufactured scaffolds for bone tissue engineering: Physical characterization of thermoplastic composites with functional fillers

Sinha R, Sanchez A, Camara-Torres M, Uriszar-Aldaca IC, Calore AR, Harings J, Gambardella A, Ciccarelli L, Vanzanella V, Sisani M, Scatto M, Wendelbo R, Perez S, Villanueva S, Matanza A, Patelli A, Grizzuti N, Mota C, and Moroni L. ACS Applied Polymer Materials 3, 3788 (2021)

3 New kinetic monte carlo model to study the dissolution of quartz

Martin P, Gaitero JJ, Dolado JS, and Manzano H. ACS Earth and Space Chemistry 5, 516 (2021)

4 Reassessing alkyne coupling reactions while studying the electronic properties of diverse pyrene linkages at surfaces

Lawrence J, Mohammed MSG, Rey D, Aguilar-Galindo F, Berdonces-Layunta A, Pena D, and De Oteyza DG. ACS Nano 15, 4937 (2021)

5 Chemical stability of (3,1)-chiral graphene nanoribbons

Berdonces-Layunta A, Lawrence J, Edalatmanesh S, Castro-Esteban J, Wang T, Mohammed MSG, Colazzo L, Pena D, Jelinek P, and De Oteyza DG. ACS Nano 15, 5610 (2021)

6 Out-of-plane transport of 1T-TaS₂/graphene-based Van der Waals heterostructures

Boix-Constant C, Manas-Valero S, Cordoba R, and Baldovi JJ. ACS Nano 15, 11898 (2021)

7 Noncollinear magnetic order in two-dimensional NiBr₂ films grown on Au(111)

Bikaljevic D, Gonzalez-Orellana C, Pena-Diaz M, Steiner D, Dreiser J, Gargiani P, Foerster M, Nino MA, Aballe L, Ruiz-Gomez S, Friedrich N, Hieulle J, Li JC, Ilyn M, Rogero C, and Pascual JL. ACS Nano 15, 14985 (2021)

8 Order from a mess: The growth of 5-armchair graphene nanoribbons

Berdonces-Layunta A, Schulz F, Aguilar-Galindo F, Lawrence J, Mohammed MSG, Muntwiler M, Lobo-Checa J, Liljeroth P, and De Oteyza DG. ACS Nano 15, 16552 (2021)

9 Mark Stockman: Evangelist for plasmonics

Aizpurua J, Atwater HA, Baumberg JJ, Bozhevolnyi SI, Brongersma ML, Dionne JA, Giessen H, Halas N, Kivshar Y, Kling MF, Krausz F, Maier S, Makarov SV, Mikkelsen M, Moskovits M, Norlander P, Odom T, Polman A, Qiu CW, Segev M, Shalaev VM, Torma P, Tsai DP, Verhagen E, Zayats A, Zhang X, and Zheludev NI. ACS Photonics 8, 683 (2021)

PUBLICATIONS

10 Effect of a dielectric spacer on electronic and electromagnetic interactions at play in molecular exciton decay at surfaces and in plasmonic gaps

Aguilar-Galindo F, Zapata-Herrera M, Diaz-Tendero S, Aizpurua J, and Borisov AG.
ACS Photonics 8, 3495 (2021)

11 Strong Rashba effect and different f-d hybridization phenomena at the surface of the heavy-fermion superconductor CeIrIn₅

Mende M, Ali K, Poelchen G, Schulz S, Mandic V, Tarasov AV, Polley C, Generalov A, Fedorov AV, Guttler M, Laubschat, C, Kliemt K, Koroteev YM, Chulkov EV, Kummer K, Krellner C, Usachov DY, and Vyalikh DV.
Advanced Electronic Materials, 2100768 (2021)

12 Polymorphism in non-fullerene acceptors based on indacenodithienothiophene

Marina S, Scaccabarozzi AD, Gutierrez-Fernandez E, Solano E, Khirbat A, Ciammaruchi L, Iturrospe A, Balzer A, Yu LY, Gabirondo E, Monnier X, Sardon H, Anthopoulos TD, Caironi M, Campoy-Quiles M, Muller C, Cangialosi D, Stingelin N, and Martin J.
Advanced Functional Materials, 2103784 (2021)

13 Nanoscale-confined terahertz polaritons in a Van der Waals crystal

De Oliveira TVAG, Norenberg T, Alvarez-Perez G, Wehmeier L, Taboada-Gutierrez J, Obst M, Hempel F, Lee EJJ, Klopf JM, Errea I, Nikitin AY, Kehr SC, Alonso-Gonzalez P, and Eng LM.
Advanced Materials 33, 2005777 (2021)

14 Anomalous high-temperature superconductivity in YH₆

Troyan IA, Semenok DV, Kvashnin AG, Sadakov AV, Sobolevskiy OA, Pudalov VM, Ivanova AG, Prakapenka VB, Greenberg E, Gavriluk AG, Lyubutin IS, Struzhkin VV, Bergara A, Errea I, Bianco R, Calandra M, Mauri F, Monacelli L, Akashi R, and Oganov AR.
Advanced Materials 33, 2006832 (2021)

15 Mn-rich MnSb₂Te₄: A topological insulator with magnetic gap closing at high Curie temperatures of 45-50 K

Wimmer S, Sanchez-Barriga J, Kuppers P, Ney A, Schierle E, Freyse F, Caha O, Michalicka J, Liebmam M, Primetzhofer D, Hoffman M, Ernst A, Otrokov MM, Bihlmayer G, Weschke E, Lake B, Chulkov EV, Morgenstern M, Bauer G, Gunther S, and Rader O.
Advanced Materials 33, 2102935 (2021)

16 Atomically-precise texturing of hexagonal boron nitride nanostripes

Ali K, Fernandez L, Kherelden MA, Makarova AA, Pis I, Bondini F, Lawrence J, De Oteyza DG, Usachov DY, Vyalikh DV, De Abajo FJG, Abd El-Fattah ZM, Ortega JE, and Schiller F.
Advanced Science 8, 2101455 (2021)

17 Self-reporting of folding and aggregation by orthogonal hantzsch luminophores within a single polymer chain

De-La-Cuesta J, Verde-Sesto E, Arbe A, and Pomposo JA.
Angewandte Chemie - International Edition 60, 3534 (2021)

18 A large starphene comprising pentacene branches

Holec J, Cogliati B, Lawrence J, Berdonces-Layunta A, Herrero P, Nagata Y, Banasiewicz M, Kozankiewicz B, Corso M, Oteyza DG, Jancarik A, and Gourdon A.
Angewandte Chemie - International Edition 60, 7752 (2021)

PUBLICATIONS

19 Bottom-up fabrication and atomic-scale characterization of triply linked, laterally pi-extended porphyrin nanotapes

Sun Q, Mateo LM, Robles R, Lorente N, Ruffieux P, Bottari G, Torres T, and Fasel R.
Angewandte Chemie - International Edition 60, 16208 (2021)

20 How aromatic are molecular nanorings? The case of a six-porphyrin nanoring

Casademont-Reig I, Guerrero-Aviles R, Ramos-Cordoba E, Torrent-Sucarrat M, and Matito E.
Angewandte Chemie - International Edition 60, 24080 (2021)

21 On-surface synthesis and collective spin excitations of a triangulene-based nanostar

Hieulle J, Castro S, Friedrich N, Vegliante A, Lara FR, Sanz S, Rey D, Corso M, Frederiksen T, Pascual JI, and Pena D.
Angewandte Chemie - International Edition 60, 25224 (2021)

22 Strong exciton-photon coupling with colloidal quantum dots in a tunable microcavity

Dovzhenko D, Lednev M, Mochalov K, Vaskan I, Samokhvalov P, Rakovich Y, and Nabiev I.
Applied Physics Letters 119, 011102 (2021)

23 Raman frequencies of diamond under non-hydrostatic pressure

Bakhit AMI, Mutisya S, and Scandolo S.
Applied Physics Letters 119, 211902 (2021)

24 Metallic carbon nanotube quantum dots with broken symmetries as a platform for tunable terahertz detection

Buchs G, Marganska M, Gonzalez JW, Eimre K, Pignedoli CA, Passerone D, Ayuela A, Groning O, and Bercieux D.
Applied Physics Reviews 8, 21406 (2021)

25 Length absence of spillover of hydrogen adsorbed on small palladium clusters anchored to graphene vacancies

Granja-DelRio A, Alducin M, Juaristi JI, Lopez MJ, and Alonso JA.
Applied Surface Science 559, 149835 (2021)

26 Digging Ti interstitials at the $r\text{-TiO}_2(110)$ surface: Mechanism of porphyrin Ti sequestration by iminic N nucleophilic attack

Kremer MK, Forrer D, Rogero C, Floreano L, and Vittadini A.
Applied Surface Science 564, 150403 (2021)

27 An epilepsy-causing mutation leads to co-translational misfolding of the Kv7.2 channel

Urrutia J, Aguado A, Gomis-Perez C, Muguruza-Montero A, Ballesteros OR, Zhang JR, Nunez E, Malo C, Chung HJ, Leonardo A, Bergara A, and Villarroel A.
BMC Biology 19, 109 (2021)

28 Emergence of dynamical disorder and phase metastability in carbon nanobowls

Gaboardi M, Silverwood I, Braunewell B, Siegel J, and Fernandez-Alonso F.
Carbon 183, 196 (2021)

PUBLICATIONS

29 Nitrogen-doped graphene on a curved nickel surface

Vilkov OY, Tarasov AV, Bokai KA, Makarova AA, Muntwiler M, Schiller F, Ortega JE, Yashina LV, Vyalikh DV, and Usachov DY.
Carbon 183, 711 (2021)

30 Mineralogical and microstructural alterations in a portland cement paste after an accelerated decalcification process

Garcia-Lodeiro I, Goracci G, Dolado JS, and Blanco-Varela MT.
Cement and Concrete Research 140, 106312 (2021)

31 Belite cements and their activation

Cuesta A, Ayuela A, and Aranda MAG.
Cement and Concrete Research 140, 106319 (2021)

32 Normal and anomalous self-healing mechanism of crystalline calcium silicate hydrates

Dupuis R, Moon J, Jeong Y, Taylor R, Kang SH, Manzano H, Ayuela A, Monteiro PJM, and Dolado JS.
Cement and Concrete Research 142, 106356 (2021)

33 A dissolution model of alite coupling surface topography and ions transport under different hydrodynamics conditions at microscale

Chen JY, Martin PB, Xu ZY, Manzano H, Dolado JS, and Ye G.
Cement and Concrete Research 142, 106377 (2021)

34 Molecular dynamics and experimental study on the adhesion mechanism of polyvinyl alcohol (PVA) fiber in alkali-activated slag/fly ash

Zhang SZ, Duque-Redondo E, Kostiuchenko A, Dolado JS, and Ye G.
Cement and Concrete Research 145, 106452 (2021)

35 Thermal noise effects on the magnetization switching of a ferromagnetic anomalous Josephson junction

Guarcello C, and Bergeret FS.
Chaos Solitons & Fractals 142, 110384 (2021)

36 Using microemulsions: Formulation based on knowledge of their mesostructure

Gradzielski M, Duvail M, De Molina PM, Simon M, Talmon Y, and Zemb T.
Chemical Reviews 121, 5671 (2021)

37 Polariton-assisted manipulation of energy relaxation pathways: Donor-acceptor role reversal in a tuneable microcavity

Dovzhenko D, Lednev M, Mochalov K, Vaskan I, Rakovich Y, Karaulov A, and Nabiev I.
Chemical Science 12, 12794 (2021)

38 Methylammonium governs structural and optical properties of hybrid lead halide perovskites through dynamic hydrogen bonding

Saleh G, Biffi G, Di Stasio F, Martin-Garcia B, Abdelhady AL, Manna L, Krahne R, and Artyukhin S.
Chemistry of Materials 33, 8524 (2021)

PUBLICATIONS

39 Correlation between the dynamics of nanoconfined water and the local chemical environment in calcium silicate hydrate nanominerals

Musumeci V, and Goracci G, Camacho PS, Dolado JS, and Aymonier C.
Chemistry- A European Journal 27, 11238 (2021)

40 Microscopic mechanism of radionuclide Cs retention in Al containing C-S-H nanopores

Duque-Redondo E, Yamada K, Dolado JS, and Manzano H.
Computational Materials Science 190, 110312 (2021)

41 Crystallization process and site-selective excitation of Nd³⁺ in LaF₃/NaLaF₄ sol-gel-synthesized transparent glass-ceramics

Cruz ME, Li J, Gorni G, Duran A, Mather GC, Balda R, Fernandez J, and Castro Y.
Crystals 11, 464 (2021)

42 Disentangling the magnetic dimensionality of an alleged magnetically isolated cuprate spin-ladder CuHpCl system: A long-lasting issue

Jornet-Somoza J, Cosi F, Fumanal M, and Deumal M.
Dalton Transactions 50, 1754 (2021)

43 Crowding effects on the structure and dynamics of the intrinsically disordered nuclear chromatin protein NUPR1

Bonucci A, Palomino-Schatzlein M, De Molina PM, Arbe A, Pierattelli R, Rizzuti B, Iovanna JL, and Neira JL.
Frontiers in Molecular Biosciences 8, 684622 (2021)

44 Reflecting laser-driven shocks in diamond in the megabar pressure range

Jakubowska K, Mancelli D, Benocci R, Trela J, Errea I, Martynenko AS, Neumayer P, Rosmej O, Borm B, Molineri A, Verona C, Cannata D, Aliverdiev A, Roman HE, and Batani D.
High Power Laser Science and Engineering 9, e3 (2021)

45 Complex networks reveal emergent interdisciplinary knowledge in Wikipedia

Schwartz GA.
Humanities & Social Sciences Communications 8, 127 (2021)

46 Structural and optical properties in Tm³⁺/Tm³⁺-Yb³⁺ doped NaLuF₄ glass-ceramics

Velazquez JJ, Balda R, Fernandez J, Gorni G, Sedano M, Duran A, Galusek D, and Pascual MJ.
International Journal of Applied Glass Science 12, 485 (2021)

47 High-surface-area organic matrix tris(aza) pentacene supported platinum nanostructures as selective electrocatalyst for hydrogen oxidation/ evolution reaction and suppressive for oxygen reduction reaction

Santa JFV, Menart S, Bele M, Ruiz-Zepeda F, Jovanovic P, Jovanovski V, Sala M, Smiljanic M, and Hodnik N.
International Journal of Hydrogen Energy 49, 25039 (2021)

48 Structural relaxation and vibrational properties of a surface with point defects

Rusina GG, Borisova SD, and Chulkov EV.
JETP Letters 114, 85 (2021)

PUBLICATIONS

49 A novel vibrational spectroscopy using spintronic-plasmonic antennas: Magneto-refractive surface-enhanced infrared absorption

Armelles G, Bergamini L, Cebollada A, Zabala N, and Aizpurua J.
Journal of Applied Physics 129, 73103 (2021)

50 From single-particle-like to interaction-mediated plasmonic resonances in graphene nanoantennas

Muller MM, Kosik M, Pelc M, Bryant GW, Ayuela A, Rockstuhl C, and Slowik K.
Journal of Applied Physics 129, 93103 (2021)

51 Quantum anharmonic enhancement of superconductivity in $P6_3/mmc$ ScH_6 at high pressures: A first-principles study

Hou PG, Belli F, Bianco R, and Errea I.
Journal of Applied Physics 130, 175902 (2021)

52 Preparation and characterization of non-vulcanized natural rubber-based cocoa pod husk composites

Edjenguele A, Alegria A, Arrese-Igor S, Ehabe EE, and Nkengafac NJ.
Journal of Applied Polymer Science 139, e51464 (2021)

53 Intermolecular interactions in optical cavities: An ab initio QED study

Haugland TS, Schafer C, Ronca E, Rubio A, and Koch H.
Journal of Chemical Physics 154, 094113 (2021)

54 Photoinduced desorption dynamics of CO from Pd(111): A neural network approach

Jimenez AS, Muzas APS, Zhang YL, Ovcara J, Jiang B, Loncaric I, Juaristi JI, and Alducin M.
Journal of Chemical Theory and Computation 17, 4648 (2021)

55 Enhancing arsenic adsorption via excellent dispersion of iron oxide nanoparticles inside poly(vinyl alcohol) nanofibers

Torasso N, Vergara-Rubio A, Rivas-Rojas P, Huck-Iriart C, Larranaga A, and Fernandez-Cirelli A.
Journal of Environmental Chemical Engineering 9, 104664 (2021)

56 Boosting background suppression in the NEXT experiment through Richardson-Lucy deconvolution

Simon A, Ifergan Y, Redwine AB, Weiss-Babai R, Arazi L, Adams C, Almazan H, Alvarez V, Aparicio B, Aranburu AI, Arnquist IJ, Azevedo CDR, Bailey K, Ballester F, Benlloch-Rodriguez JM, Borges FIGM, Byrnes N, Carcel S, Carrion JV, Cebrian S, Church E, Conde CAN, Contreras T, Cossio FP, Denisenko AA, Diaz G, Diaz J, Escada J, Esteve R, Felkai R, Fernandes LMP, Ferrario P, Ferreira AL, Foss F, Freitas EDC, Freixa Z, Generowicz J, Goldschmidt A, Gomez-Cadenas JJ, Gonzalez R, Gonzalez-Diaz D, Gosh S, Guenette R, Gutierrez RM, Haefner J, Hafidi K, Hauptman J, Henriques CAO, Morata JAH, Herrero P, Herrero V, Ho J, Jones BJP, Kekic M, Labarga L, Laing A, Lebrun P, Lopez-March N, Losada M, Mano RDP, Martin-Albo J, Martinez A, Martinez-Vara M, Martinez-Lema G, McDonald AD, Meziani ZE, Monrabal F, Monteiro, CMB, Mora FJ, Vidal JM, Newhouse C, Novella P, Nygren DR, Oblak E, Odriozola-Gimeno M, Palmeiro B, Para A, Perez J, Querol M, Renner J, Ripoll L, Rivilla I, Garcia YR, Rodriguez J, Rogero C, Rogers L, Romeo B, Romo-Luque C, Santos FP, dos Santos JMF, Sorel M, Stanford C, Teixeira JMR, Thapa P, Toledo JF, Torrent J, Uson A, Veloso JFCA, Vuong TT, Webb R, White JT, Woodruff K, and Yahlali N.
Journal of High Energy Physics 7, 146 (2021)

57 Sensitivity of a tonne-scale NEXT detector for neutrinoless double-beta decay searches

Adams C, Alvarez V, Arazi L, Arnquist IJ, Azevedo CDR, Bailey K, Ballester F, Benlloch-Rodriguez JM, Borges FIGM, Byrnes N, Carcel S, Carrion JV, Cebrian S, Church E, Conde CAN, Contreras T, Denisenko AA, Diaz G, Diaz J, Escada J, Esteve R, Felkai R, Fernandes LMP, Ferrario P, Ferreira AL, Foss F, Freitas EDC, Freixa Z, Generowicz J, Goldschmidt A, Gomez-Cadenas JJ, Gonzalez R, Gonzalez-Diaz D, Gosh S, Guenette R, Gutierrez RM, Haefner J, Hafidi K, Hauptman J, Henriques CAO, Morata JAH, Herrero P, Herrero V, Ifergan Y, Jones BJP, Kekic M, Labarga L, Laing A, Lebrun P, Lopez-March N, Losada M, Mano RDP, Martin-Albo J, Martinez A, Martinez-Vara M, Martinez-Lema G, McDonald AD, Meziani ZE, Monrabal F, Monteiro CMB, Mora FJ, Vidal JM, Newhouse C, Novella P, Nygren DR, Oblak E, Palmeiro B, Para A, Perez J, Querol M, Redwine A, Renner J, Ripoll L, Rivilla I, Garcia YR, Rodriguez J, Rogero C, Rogers L, Romeo B, Romo-Luque C, Santos FP, dos Santos JMF, Simon A, Sorel M, Stanford C, Teixeira JMR, Thapa P, Toledo JF, Torrent J, Uson A, Veloso JFCA, Vuong TT, Webb R, Weiss-Babai R, White JT, Woodruff K, and Yahlali N. *Journal of High Energy Physics* 8, 164 (2021)

58 Nd³⁺-doped- SiO₂-KLaF₄ oxyfluoride glass-ceramics prepared by sol-gel

Cruz ME, Li J, Gorni G, Duran A, Mather GC, Balda R, Fernandez J, and Castro Y. *Journal of Luminescence* 235, 118035 (2021)

59 High-dimensional atomistic neural network potential to study the alignment-resolved O₂ scattering from highly oriented pyrolytic graphite

Santamaria AR, Ramos M, Alducin M, Busnengo HF, Muino RD, and Juaristi JI. *Journal of Physical Chemistry A* 125, 2588 (2021)

60 Light-induced charge transfer from transition-metal-doped aluminum clusters to carbon dioxide

Gobel A, Rubio A, and Lischner J. *Journal of Physical Chemistry A* 125, 5878 (2021)

61 Persistence of the topological surface states in Bi₂Se₃ against Ag intercalation at room temperature

Ye M, Kuroda K, Otrokov MM, Ryabishchenkova AG, Jiang Q, Ernst A, Chulkov EV, Nakatake M, Arita M, Okuda T, Matsushita T, Toth L, Daimon H, Shimada K, Ueda Y, and Kimura A. *Journal of Physical Chemistry C* 125, 1784 (2021)

62 pH-sensing platform based on light-matter coupling in colloidal complexes of silver nanoplates and J-aggregates

Krivenkov V, Samokhvalov P, Nabiev I, and Rakovich YP. *Journal of Physical Chemistry C* 125, 1972 (2021)

63 Hydrated alkali atoms on Copper(111): A density functional theory study

Paz AP, and Rubio A. *Journal of Physical Chemistry C* 125, 3868 (2021)

64 Why a good catalyst can turn out detrimental to good polymerization

Abadia M, Brede J, Verdini A, Floreano L, Nita P, De Oteyza DG, Ortega JE, Corso M, and Rogero C. *Journal of Physical Chemistry C* 125, 5066 (2021)

65 Mapping of guest localization in mesoporous silica particles by solid-state NMR and ab initio modeling: New insights into benzoic acid and p-fluorobenzoic acid embedded in MCM-41 via ball milling

Trzeciak K, Kazmierski S, Druzicki K, and Potrzebowski MJ.
Journal of Physical Chemistry C 125, 10096 (2021)

66 Insights into the coadsorption and reactivity of O and CO on Ru(0001) and their coverage dependence

Tetenoire A, Juaristi JI, and Alducin M.
Journal of Physical Chemistry C 125, 12614 (2021)

67 Lateral interactions and order-disorder phase transitions of metal phthalocyanines on Ag(111)

Fernandez L, Thussing S, Brion-Rios AX, Sanchez-Portal D, and Jakob P.
Journal of Physical Chemistry C 125, 15623 (2021)

68 Interplay between local structure and nuclear dynamics in tungstic acid: A neutron scattering study

Lalik E, Druzicki K, Irvine G, Gutmann M, Rudic S, Manuel P, Petricek V, and Krzystyniak M.
Journal of Physical Chemistry C 125, 23864 (2021)

69 Spectroscopic signatures of hydrogen-bonding motifs in protonic ionic liquid systems: Insights from diethylammonium nitrate in the solid state

Vazquez-Fernandez I, Druzicki K, Fernandez-Alonso F, Mukhopadhyay S, Nockemann P, Parker SF, Rudic S, Stana SM, Tomkinson J, Yeadon DJ, Seddon KR, and Plechkova NV.
Journal of Physical Chemistry C 125, 24463 (2021)

70 Dominant role of quantum anharmonicity in the stability and optical properties of infinite linear acetylenic carbon chains

Romanin D, Monacelli L, Bianco R, Errea I, Mauri F, and Calandra M.
Journal of Physical Chemistry Letters 12, 10339 (2021)

71 Superconducting scanning tunneling microscope tip to reveal sub-millielectronvolt magnetic energy variations on surfaces

Mier C, Verlhac B, Gamier L, Robles R, Limot L, Lorente N, and Choi DJ.
Journal of Physical Chemistry Letters 12, 2983 (2021)

72 Simulating vibronic spectra without Born-Oppenheimer surfaces

Lively K, Albareda G, Sato SA, Kelly A, and Rubio A.
Journal of Physical Chemistry Letters 12, 3074 (2021)

73 Cation dynamics and structural stabilization in formamidinium lead iodide perovskites

Druzicki K, Laven R, Armstrong J, Malavasi L, Fernandez-Alonso F, and Karlsson M.
Journal of Physical Chemistry Letters 12, 3503 (2021)

74 Molecular transistor controlled through proton transfer

Weckbecker D, Coto PB, and Thoss M.
Journal of Physical Chemistry Letters 12, 413 (2021)

PUBLICATIONS

75 Ba with unusual oxidation states in Ba chalcogenides under pressure

Li F, Zhang XH, Fu Y, Wang YC, Bergara A, and Yang GC.
Journal of Physical Chemistry Letters 12, 4203 (2021)

76 Topological magnetic materials of the $(\text{MnSb}_2\text{Te}_4)_n(\text{Sb}_2\text{Te}_3)_n$ Van der Waals compounds family

Eremeev SV, Rusinov IP, Koroteev YM, Vyazovskaya AY, Hoffmann M, Echenique PM, Ernst A, Otrokov MM, and Chulkov EV.
Journal of Physical Chemistry Letters 12, 4268 (2021)

77 Anisotropic and high-mobility C_3S monolayer as a photocatalyst for water splitting

Tang M, Wang B, Lou H, Li F, Bergara A, and Yang GC.
Journal of Physical Chemistry Letters 12, 8320 (2021)

78 Insight into the temperature evolution of electronic structure and mechanism of exchange interaction in EuS

Fedorov AV, Poelchen G, Eremeev SV, Schulz S, Generalov A, Polley C, Laubschat C, Kliemt K, Kaya N, Krellner C, Chulkov EV, Kummer K, Usachov DY, Ernst A, and Vyalikh DV.
Journal of Physical Chemistry Letters 12, 8328 (2021)

79 Wide band gap P_3S monolayer with anisotropic and ultrahigh carrier mobility

Wang B, Tang M, Lou H, Li F, Bergara A, and Yang GC.
Journal of Physical Chemistry Letters 12, 8481 (2021)

80 Reduced carbon monoxide saturation coverage on vicinal palladium surfaces: The importance of the adsorption site

Garcia-Martinez F, Dietze E, Schiller F, Gajdek D, Merte LR, Gericke SM, Zetterberg J, Albertin S, Lundgren E, Gronbeck H, and Ortega JE.
Journal of Physical Chemistry Letters 12, 9508 (2021)

81 Semiconducting MnB_5 monolayer as a potential photovoltaic material

Han FJJ, Yu T, Qu X, Bergara A, and Yang GC.
Journal of Physics-Condensed Matter 33, 175702 (2021)

82 Magnetic correlations in single-layer NbSe_2

Divilov S, Wan W, Dreher P, Bolen E, Sanchez-Portal D, Ugeda MM, and Yndurain F.
Journal of Physics-Condensed Matter 33, 295804 (2021)

83 The stochastic self-consistent harmonic approximation: Calculating vibrational properties of materials with full quantum and anharmonic effects

Monacelli L, Bianco R, Cherubini M, Calandra M, Errea I, and Mauri F.
Journal of Physics-Condensed Matter 33, 363001 (2021)

84 Theoretical treatment of single-molecule scanning Raman picoscopy in strongly inhomogeneous near fields

Zhang Y, Dong ZC, and Aizpurua J.
Journal of Raman Spectroscopy 52, 296 (2021)

PUBLICATIONS

85 Rheological and thermal properties of purified raw natural rubber

Nkayem DEN, Alegria A, Arrese-Igor S, and Nkengafac NJ.
Journal of Rubber Research 24, 709 (2021)

86 Nonadiabatic localization of H₂ in the field of two external positive tip charges

Schattke W, Van Hove MA, and Muino RD.
Journal of Vacuum Science & Technology A 39, 053206 (2021)

87 Multiple Kerker anapoles in dielectric microspheres

Sanz-Fernandez C, Molezuelas-Ferreras M, Lasa-Alonso J, De Sousa N, Zambrana-Puyalto X, and Olmos-Trigo J.
Laser & Photonics Reviews 15, 2100035 (2021)

88 Shock hugoniot data for water up to 5 Mbar obtained with quartz standard at high-energy laser facilities

Errea I, Tentori A, Turianska O, Larreur H, Katagiri K, Ozaki N, Kamimura N, Kamibayashi D, Ishida K, Ogura H, Kawasaki K, Maeda Y, Hironaka Y, Shigemori Y, Batani K, Schaumann G, Rosmej O, Neumayer P, Zielbauer B, Martynenko AS, Filippov ED, Pikuz S, and Batani D.
Lasers and Particle Beams 2021, 4141522 (2021)

89 Cationic polymerization of beta-pinene using B(C₆F₅)₃ as a Lewis acid for the synthesis of tackifiers in pressure sensitive adhesives

Destephen A, Roman EGD, Martinez-Tong DE, and Ballard N.
Macromolecular Materials and Engineering 306, 2100194 (2021)

90 Triggering forces at the nanoscale: Technologies for single-chain mechanical activation and manipulation

Martinez-Tong DE, Pomposo JA, and Verde-Sesto E.
Macromolecular Rapid Communications 42, 2000654 (2021)

91 Mapping chemical structure-glass transition temperature relationship through artificial intelligence

Miccio LA, and Schwartz GA.
Macromolecules 54, 1811 (2021)

92 Enhanced free surface mobility facilitates the release of free volume holes in thin-film polymer glasses

Zha H, Wang Q, Wang XP, Cangialosi D, and Zuo B.
Macromolecules 54, 2022 (2021)

93 Non-Einstein rheology in segmented polyurethane nanocomposites

Heydarnezhad HR, Mohammadi N, and Alegria A.
Macromolecules 54, 2783 (2021)

94 Gel formation in reversibly cross-linking polymers

Formanek M, Rovigatti L, Zaccarelli E, Sciortino F, and Moreno AJ.
Macromolecules 54, 6613 (2021)

PUBLICATIONS

95 Direct visualization and characterization of interfacially adsorbed polymer atop nanoparticles and within nanocomposites

Randazzo K, Bartkiewicz M, Graczykowski B, Cangialosi D, Fytas G, Zuo BA, and Priestley RD.
Macromolecules 54, 10224 (2021)

96 Basalt fibre surface modification via plasma polymerization of tetravinylsilane/oxygen mixtures for improved interfacial adhesion with unsaturated polyester matrix

Lilli M, Jurko M, Sirjovova V, Zvonek M, Cech V, Scheffler C, Rogero C, Ilyn M, Tirillo J, and Sarasini F.
Materials Chemistry and Physics 274, 125106 (2021)

97 Significant effect of intra-chain distribution of catalytic sites on catalytic activity in "clickase" single-chain nanoparticles

Asenjo-Sanz I, Claros T, Gonzalez E, Pinacho-Olaciregui J, Verde-Sesto E, and Pomposo JA.
Materials Letters 304, 130622 (2021)

98 Phase transitions of alkaline-earth metal sulfides under pressure

Wang YF, Bergara A, Shao CC, Wang L, Liang XW, Wang LY, Sun RX, Wei XD, Wang TS, and Gao GY.
Materials Research Express 8, 065902 (2021)

99 Size effects in finite element modelling of 3D printed bone scaffolds using hydroxyapatite PEOT/PBT composites

Calderon-Uriszar-Aldaca I, Perez S, Sinha R, Camara-Torres M, Villanueva S, Mota C, Patelli A, Matanza A, Moroni L, and Sanchez A.
Mathematics 9, 1746 (2021)

100 Tailoring superconductivity in large-area single-layer NbSe₂ via self-assembled molecular adlayers

Calavalle F, Dreher P, Surdendran AP, Wan W, Timpel M, Verucchi R, Rogero C, Bauch T, Lombardi F, Casanova F, Nardi MV, Ugeda MM, Hueso LE, and Gobbi M.
Nano Letters 21, 136 (2021)

101 Toward confined carbyne with tailored properties

Shi L, Senga R, Suenaga K, Kataura H, Saito T, Paz AP, Rubio A, Ayala P, and Pichler T.
Nano Letters 21, 1096 (2021)

102 Survival of floquet-bloch states in the presence of scattering

Aeschlimann S, Sato SA, Krause R, Chavez-Cervantes M, De Giovannini U, Hubener H, Forti S, Coletti C, Hanff K, Rossnagel K, Rubio A, and Gierz I.
Nano Letters 21, 5028 (2021)

103 Electronic temperature and two-electron processes in overbias plasmonic emission from tunnel junctions

Martin-Jimenez A, Lauwaet K, Jover O, Granados D, Arnau A, Silkin VM, Miranda R, and Otero R.
Nano Letters 21, 7086 (2021)

PUBLICATIONS

104 Engineering three-dimensional Moire flat bands

Xian LD, Fischer A, Claassen M, Zhang J, Rubio A, and Kennes DM.
Nano Letters 21, 7519 (2021)

105 Doublet-singlet-doublet transition in a single organic molecule magnet on-surface constructed with up to 3 aluminum atoms

Soe WH, Robles R, De Mendoza P, Echavarren AM, Lorente N, and Joachim C.
Nano Letters 21, 8317 (2021)

106 Electronic exciton-plasmon coupling in a nanocavity beyond the electromagnetic interaction picture

Babaze A, Esteban R, Borisov AG, and Aizpurua J.
Nano Letters 21, 8466 (2021)

107 Fast intrinsic emission quenching in Cs₄PbBr₆ nanocrystals

Petralanda U, Biffi G, Boehme SC, Baranov D, Krahne R, Manna L, and Infante I.
Nano Letters 21, 8619 (2021)

108 Interactions between reduced graphene oxide with monomers of (calcium) silicate hydrates: A first-principles study

Izadifar M, Dolado JS, Thissen P, and Ayuela A.
Nanomaterials 11, 2248 (2021)

109 Band structure and energy level alignment of chiral graphene nanoribbons on silver surfaces

Corso M, Menchon RE, Piquero-Zulaica I, Vilas-Varela M, Ortega JE, Pena D, Garcia-Lekue A, and De Oteyza DG.
Nanomaterials 11, 3303 (2021)

110 Single-nanoantenna driven nanoscale control of the VO₂ insulator to metal transition

Bergamini L, Chen BG, Traviss D, Wang YD, De Groot CH, Gaskell JM, Sheel DW, Zabala N, Aizpurua J, and Muskens OL.
Nanophotonics 10, 3745 (2021)

111 Addressing molecular optomechanical effects in nanocavity-enhanced Raman scattering beyond the single plasmonic mode

Zhang Y, Esteban R, Boto RA, Urbieto M, Arrieta X, Shan CX, Li SZ, Baumberg JJ, and Aizpurua J.
Nanoscale 13, 1938 (2021)

112 Strong increase in the effective two-photon absorption cross-section of excitons in quantum dots due to the nonlinear interaction with localized plasmons in gold nanorods

Krivenkov V, Samokhvalov P, Sanchez-Iglesias A, Grzelczak M, Nabiev I, and Rakovich Y. Nanoscale 13, 4614 (2021)

113 Searching for kagome multi-bands and edge states in a predicted organic topological insulator

Hernandez-Lopez L, Piquero-Zulaica I, Downing CA, Piantek M, Fujii J, Serrate D, Ortega JE, Bartolome F, and Lobo-Checa J.
Nanoscale 13, 5216 (2021)

PUBLICATIONS

114 Coupling plasmonic catalysis and nanocrystal growth through cyclic regeneration of NADH

Sanchez-Iglesias A, Kruse J, Chuvilin A, and Grzelczak M.
Nanoscale 13, 15188 (2021)

115 Power discontinuity and shift of the energy onset of a molecular de-bromination reaction induced by hot-electron tunneling

Barragan A, Robles R, Lorente N, and Vitali L.
Nanoscale 13, 15215 (2021)

116 One-way rotation of a chemically anchored single molecule-rotor

Eisenhut F, Kuhne T, Monsalve J, Srivastava S, Ryndyk DA, Cuniberti G, Aiboudi O, Lissel F, Zobac V, Robles R, Lorente N, Joachim C, and Moresco F.
Nanoscale 13, 16077 (2021)

117 Ultrafast demagnetization in a ferrimagnet under electromagnetic field funneling

Mishra K, Ciuciulkaite A, Zapata-Herrera M, Vavassori P, Kapaklis V, Rasing T, Dmitriev A, Kimel A, and Kirilyuk A.
Nanoscale 13, 19367 (2021)

118 Plasmon-exciton interaction strongly increases the efficiency of a quantum dot-based near-infrared photodetector operating in the two-photon absorption mode under normal conditions

Krivenkov V, Samokhvalov P, Vasil'evskii IS, Kargin NI, and Nabiev I.
Nanoscale 13, 19929 (2021)

119 From starphenes to non-benzenoid linear conjugated polymers by substrate templating

Mohammed MSG, Lawrence J, Garcia F, Brandimarte P, Berdonces-Layunta A, Perez D, Sanchez-Portal D, Pena D, and De Oteyza DG.
Nanoscale Advances 3, 2351 (2021)

120 Magnetism found in zigzag graphene nanoribbons

Garcia-Lekue A, and Sánchez-Portal D.
Nature (News & Views) 600, 613 (2021)

121 Van der Waals driven anharmonic melting of the 3D charge density wave in VSe₂

Diego J, Said AH, Mahatha SK, Bianco R, Monacelli L, Calandra M, Mauri F, Rossmagel K, Errea I, and Blanco-Canosa S.
Nature Communications 12, 598 (2021)

122 Unravelling the intertwined atomic and bulk nature of localised excitons by attosecond spectroscopy

Lucchini M, Sato SA, Lucarelli GD, Moio B, Inzani G, Borrego-Varillas R, Frassetto F, Poletto L, Hubener H, De Giovannini U, Rubio A, and Nisoli M.
Nature Communications 12, 1021 (2021)

PUBLICATIONS

123 Complex plasmon-exciton dynamics revealed through quantum dot light emission in a nanocavity

Gupta SN, Bitton O, Neuman T, Esteban R, Chuntanov L, Aizpurua J, and Haran G.
Nature Communications 12, 1310 (2021)

124 Coherent coupling between vortex bound states and magnetic impurities in 2D layered superconductors

Park S, Barrena V, Manas-Valero S, Baldovi JJ, Fente A, Herrera E, Mompean F, Garcia-Hernandez M, Rubio A, Coronado E, Guillaumon I, Yeyati AL, and Suderow H.
Nature Communications 12, 4668 (2021)

125 Reconfigurable artificial microswimmers with internal feedback

Alvarez L, Fernandez-Rodriguez MA, Alegria A, Arrese-Igor S, Zhao K, Kroger M, and Isa L.
Nature Communications 12, 4762 (2021)

126 Strong correlation between electronic bonding network and critical temperature in hydrogen-based superconductors

Belli F, Novoa T, Contreras-Garcia J, and Errea I.
Nature Communications 12, 5381 (2021)

127 Topological phase transition in chiral graphene nanoribbons: From edge bands to end states

Li JC, Sanz S, Merino-Diez N, Vilas-Varela M, Garcia-Lekue A, Corso M, De Oteyza DG, Frederiksen T, Pena D, and Pascual JI.
Nature Communications 12, 5538 (2021)

128 Microcavity phonon polaritons from the weak to the ultrastrong phonon-photon coupling regime

Barra-Burillo M, Muniain U, Catalano S, Autore M, Casanova F, Hueso LE, Aizpurua J, Esteban R, and Hillenbrand R.
Nature Communications 12, 6206 (2021)

129 Quantitative sampling of atomic-scale electromagnetic waveforms

Peller D, Roelcke C, Kastner LZ, Buchner T, Neef A, Hayes J, Bonafe F, Sidler D, Ruggenthaler M, Rubio A, Huber R, and Repp J.
Nature Photonics 15, 143 (2021)

130 Black metal hydrogen above 360 GPa driven by proton quantum fluctuations

Monacelli L, Errea I, and Calandra M.
Nature Physics 17, 63 (2021)

131 Moire heterostructures as a condensed-matter quantum simulator

Kennes DM, Claassen M, Xian LD, Georges A, Millis AJ, Hone J, Dean CR, Basov DN, Pasupathy AN, and Rubio A.
Nature Physics 17, 155 (2021)

132 GW approximation for open-shell molecules: A first-principles study

Mansouri M, Casanova D, Koval P, and Sanchez-Portal D.
New Journal of Physics 23, 093027 (2021)

PUBLICATIONS

133 Energy test of an efficient random laser emission collecting system

Iparraguirre I, Azkargorta J, Fernandez J, Garcia-Revilla S, and Balda R.
Optical Engineering 60, 010502 (2021)

134 Bandwidth control of the biphoton wavefunction exploiting spatio-temporal correlations

Varga JJM, Lasa-Alonso J, Molezuelas-Ferreras M, Tischler N, and Molina-Terriza G.
Optics Communications 504, 127461 (2021)

135 Hybrid photonic-plasmonic cavities based on the nanoparticle-on-a-mirror configuration

Barreda AI, Zapata-Herrera M, Palstra IM, Mercade L, Aizpurua J, and Koenderink AF.
Photonics Research 9, 2398 (2021)

136 Transformation of a graphene nanoribbon into a hybrid 1D nanoobject with alternating double chains and polycyclic regions

Sinitisa AS, Lebedeva IV, Polynskaya YG, De Oteyza DG, Ratkevich SV, Knizhnik AA, Popov AM, Poklonski NA, and Lozovik YE.
Physical Chemistry Chemical Physics 23, 425 (2021)

137 The formation and migration of non-equivalent oxygen vacancies in $\text{PrBaCo}_{2-x}\text{M}_x\text{O}_{6-\delta}$, where M = Fe, Co, Ni and Cu

Zhukov VP, Chulkov EV, Politov BV, Suntsov AY, and Kozhevnikov VL.
Physical Chemistry Chemical Physics 23, 2313 (2021)

138 Magnetic and vibrational properties of small chromium clusters on the Cu(111) surface

Borisova SD, Ereemeev SV, Rusina GG, and Chulkov EV.
Physical Chemistry Chemical physics 23, 7814 (2021)

139 Ab initio molecular dynamics of hydrogen on tungsten surfaces

Rodriguez-Fernandez A, Bonnet L, Larregaray P, and Muino RD.
Physical Chemistry Chemical Physics 23, 7919 (2021)

140 Electron-phonon interaction in In-induced structures on Si(111) from first-principles

Sklyadneva IY, Heid R, Echenique PM, and Chulkov EV.
Physical Chemistry Chemical Physics 23, 7955 (2021)

141 Challenges in the synthesis of corannulene-based non-planar nanographenes on Au(111) surfaces

Wang T, Lawrence J, Sumi N, Robles R, Castro-Esteban J, Rey D, Mohammed MSG, Berdonces-Layunta A, Lorente N, Perez D, Pena D, Corso M, and De Oteyza DG.
Physical Chemistry Chemical Physics 23, 10845 (2021)

142 Dynamics of aqueous peptide solutions in folded and disordered states examined by dynamic light scattering and dielectric spectroscopy

Melillo JH, Gabriel JP, Pabst F, Blochowicz T, and Cervený S.
Physical Chemistry Chemical Physics 23, 15020 (2021)

PUBLICATIONS

143 The charge transport mechanism in a new magnetic topological insulator $\text{MnBi}_{0.5}\text{Sb}_{1.5}\text{Te}_4$

Abdullayev NA, Aliguliyeva KV, Zverev VN, Aliev ZS, Amiraslanov IR, Babanly MB, Jahangirli ZA, Aliyeva YN, Akhmedova KN, Mammadov TG, Otrokov MM, Shikin AM, Mamedov NT, and Chulkov EV.
Physics of the Solid State 63, 1120 (2021)

144 Finite-range effects in the two-dimensional repulsive Fermi polaron

Bombin R, Cikojevic V, Sanchez-Baena J, and Boronat J.
Physical Review A 103, L041302 (2021)

145 Experimental characterization of quantum processes: A selective and efficient method in arbitrary finite dimensions

Stefano QP, Perito I, Varga JJM, Rebon L, and Lemmi C.
Physical Review A 103, 052438 (2021)

146 First law of quantum thermodynamics in a driven open two-level system

Juan-Delgado A, and Chenu A.
Physical Review A 104, 022219 (2021)

147 High harmonics and isolated attosecond pulses from MgO

Nourbakhsh Z, Tancogne-Dejean N, Merdji H, and Rubio A.
Physical Review Applied 15, 014013 (2021)

148 Electron-phonon coupling in the magnetic Weyl semimetal ZrCo_2Sn

Sklyadneva IY, Heid R, Echenique PM, and Chulkov EV.
Physical Review B 103, 024303 (2021)

149 Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential

Yang QP, Lv J, Tong QC, Du X, Wang YC, Zhang ST, Yang GC, Bergara A, and Ma YM.
Physical Review B 103, 024505 (2021)

150 Classical and cubic Rashba effect in the presence of in-plane 4f magnetism at the iridium silicide surface of the antiferromagnet GdIr_2Si_2

Schulz S, Vyazovskaya AY, Poelchen G, Generalov A, Guttler M, Mende M, Danzenbacher S, Otrokov MM, Balasubramanian T, Polley C, Chulkov EV, Laubschat C, Peters M, Kliemt K, Krellner C, Usachov DY, and Vyalikh DV.
Physical Review B 103, 035123 (2021)

151 Quadrupole moments, edge polarizations, and corner charges in the Wannier representation

Ren S, Souza I, and Vanderbilt D.
Physical Review B 103, 035147 (2021)

152 Surface plasmons on $\text{Pd}(110)$: An *ab initio* calculation

Muniain U, Esteban R, Chernov IP, Aizpurua J, and Silkin VM.
Physical Review B 103, 045407 (2021)

PUBLICATIONS

153 Gap inversion in quasi-one-dimensional Andreev crystals

Rouco M, Bergeret FS, and Tokatly IV.
Physical Review B 103, 064505 (2021)

154 Effect of Rashba splitting on ultrafast carrier dynamics in BiTeI

Ketterl AS, Andres B, Polverigiani M, Voroshnin V, Gahl C, Kokh KA, Tereshchenko OE, Chulkov EV, Shikin A, and Weinelt M.
Physical Review B 103, 085406 (2021)

155 Strong anharmonic and quantum effects in $Pm\bar{3}n$ AlH_3 under high pressure: A first-principles study

Hou PG, Belli F, Bianco R, and Errea I.
Physical Review B 103, 134305 (2021)

156 Time-dependent forces between a swift electron and a small nanoparticle within the dipole approximation

Castrejon-Figueroa J, Castellanos-Reyes JA, Maciel-Escudero C, Reyes-Coronado A, and Barrera RG.
Physical Review B 103, 155413 (2021)

157 Quantum network approach to spin interferometry driven by Abelian and non-Abelian fields

Hijano A, van den Berg TL, Frustaglia D, and Bercioux D.
Physical Review B 103, 155419 (2021)

158 Reference plane for the electronic states in thin films on stepped surfaces

Moras P, Montes TO, Schiller F, Ferrari L, Topwal D, Locatelli A, Sheverdyayeva PM, and Carbone C.
Physical Review B 103, 165426 (2021)

159 Electronic structure and coexistence of superconductivity with magnetism in $RbEuFe_4As_4$

Kim TK, Pervakov KS, Evtushinsky DV, Jung SW, Poelchen G, Kummer K, Vlasenko VA, Sadakov AV, Usoltsev AS, Pudalov VM, Roditchev D, Stolyarov VS, Vyalikh DV, Borisov V, Valenti R, Ernst A, Ereemeev SV, and Chulkov EV.
Physical Review B 103, 174517 (2021)

160 Mirror Chern numbers in the hybrid Wannier representation

Rauch T, Olsen T, Vanderbilt D, and Souza I.
Physical Review B 103, 195103 (2021)

161 Many-body physics in small systems: Observing the onset and saturation of correlation in linear atomic chains

Townsend E, Neuman T, Debrecht A, Aizpurua J, and Bryant GW.
Physical Review B 103, 195429 (2021)

162 Domain wall induced spin-polarized flat bands in antiferromagnetic topological insulators

Petrov EK, Men'shov VN, Rusinov IP, Hoffmann M, Ernst A, Otrokov MM, Dugaev VK, Menshchikova TV, and Chulkov EV.
Physical Review B 103, 235142 (2021)

PUBLICATIONS

163 Infrared study of the multiband low-energy excitations of the topological antiferromagnet MnBi_2Te_4

Xu B, Zhang Y, Alizade EH, Jahangirli ZA, Lyzwa F, Sheveleva E, Marsik P, Li YK, Yao YG, Wang ZW, Shen B, Dai YM, Kataev V, Otrokov MM, Chulkov EV, Mamedov NT, and Bernhard C.

Physical Review B 103, L121103 (2021)

164 $\beta\text{-As}_2\text{Te}_3$: Pressure-induced three-dimensional Dirac semimetal with ultralow room-pressure lattice thermal conductivity

Da Silva EL, Leonardo A, Yang T, Santos MC, Vilaplana R, Gallego-Parra S, Bergara A, and Manjon FJ.

Physical Review B 104, 024103 (2021)

165 Spectral features of magnetic domain walls on the surface of three-dimensional topological insulators

Rusinov IP, Men'shov VN, and Chulkov EV.

Physical Review B 104, 035411 (2021)

166 Atomic manipulation of in-gap states in the beta- Bi_2Pd superconductor

Mier C, Hwang J, Kim J, Bae Y, Nabeshima F, Imai Y, Maeda A, Lorente N, Heinrich A, and Choi DJ.

Physical Review B 104, 045406 (2021)

167 Spectral properties of Andreev crystals

Rouco M, Bergeret FS, and Tokatly IV.

Physical Review B 104, 064506 (2021)

168 Magnetoelectric effects in superconductors due to spin-orbit scattering: Nonlinear sigma-model description

Virtanen P, Bergeret FS, and Tokatly IV.

Physical Review B 104, 064515 (2021)

169 Sample-dependent Dirac-point gap in MnBi_2Te_4 and its response to applied surface charge: A combined photoemission and *ab initio* study

Shikin AM, Estyunin DA, Zaitsev NL, Glazkova D, Klimovskikh II, Filnov SO, Rybkin AG, Schwier EF, Kumar S, Kimura A, Mamedov N, Aliev Z, Babanly MB, Kokh K, Tereshchenko OE, Otrokov MM, Chulkov EV, Zvezdin KA, and Zvezdin AK.

Physical Review B 104, 115168 (2021)

170 Progress towards understanding ultranonlocality through the wave-vector and frequency dependence of approximate exchange-correlation kernels

Nepal NK, Kaplan AD, Pitarke JM, and Ruzsinszky A.

Physical Review B 104, 125112 (2021)

171 Paramagnetic spin Hall magnetoresistance

Oyanagi K, Gomez-Perez JM, Zhang XP, Kikkawa T, Chen Y, Sagasta E, Chuvilin A, Hueso LE, Golovach VN, Bergeret FS, Casanova F, and Saitoh E.

Physical Review B 104, 134428 (2021)

172 Prediction of high-T-c superconductivity in ternary lanthanum borohydrides

Liang XW, Bergara A, Wei XD, Song XX, Wang LY, Sun RX, Liu HY, Hemley RJ, Wang L, Gao GY, and Tian YJ.

Physical Review B 104, 134501 (2021)

PUBLICATIONS

173 Pressure-induced superconductivity in Li-Te electrides

Zhang XH, Li F, Bergara A, and Yang GC.
Physical Review B 104, 134505 (2021)

174 Ever-present Majorana bound state in a generic one-dimensional superconductor with odd number of Fermi surfaces

Kharitonov M, Hankiewicz EM, Trauzettel B, and Bergeret FS.
Physical Review B 104, 134516 (2021)

175 Asymptotics of the metal-surface Kohn-Sham exact exchange potential revisited

Horowitz CM, Proetto CR, and Pitarke JM.
Physical Review B 104, 155108 (2021)

176 Spin resonance amplitude and frequency of a single atom on a surface in a vector magnetic field

Kim J, Jang WJ, Bui TH, Choi DJ, Wolf C, Delgado F, Chen Y, Krylov D, Lee S, Yoon S, Lutz CP, Heinrich AJ, and Bae Y.
Physical Review B 104, 174408 (2021)

177 Large spin-charge interconversion induced by interfacial spin-orbit coupling in a highly conducting all-metallic system

Pham VT, Yang HZ, Choi WY, Marty A, Groen I, Chuvilin A, Bergeret FS, Hueso LE, Tokatly IV, and Casanova F.
Physical Review B 104, 184410 (2021)

178 Validity of the on-site spin-orbit coupling approximation

Cuadrado R, Robles R, Garcia A, Pruneda M, Ordejon P, Ferrer J, and Cerda JI.
Physical Review B 104, 195104 (2021)

179 Electron-phonon coupling of Fe-adatom electron states on MgO/Ag(100)

Garai-Marin H, Ibanez-Azpiroz J, Garcia-Goiricelaya P, Gurtubay IG, and Eiguren A.
Physical Review B 104, 195422 (2021)

180 Anomalous Andreev interferometer: Study of an anomalous Josephson junction coupled to a normal wire

Hijano A, Ilic S, and Bergeret FS.
Physical review B 104, 214515 (2021)

181 Calculations of in-gap states of ferromagnetic spin chains on s-wave wide-band superconductors

Mier C, Choi DJ, and Lorente N.
Physical Review B 104, 245415 (2021)

182 All-electric electron spin resonance studied by means of Floquet quantum master equations

Reina-Galvez J, Lorente N, Delgado F, and Arrachea L.
Physical Review B 104, 245435 (2021)

183 Quantum paraelectric phase of SrTiO₃ from first principles

Shin D, Latini S, Schafer C, Sato SA, De Giovannini U, Hubener H, and Rubio A.
Physical Review B 104, L060103 (2021)

PUBLICATIONS

184 Higher-order band topology in twisted Moire superlattice

Liu B, Xian LD, Mu HM, Zhao G, Liu Z, Rubio A, and Wang ZF.

Physical Review Letters 126, 066401 (2021)

185 Self-consistent potential correction for charged periodic systems

Da Silva MC, Lorke M, Aradi B, Tabriz MF, Frauenheim T, Rubio A, Rocca D, and Deak P.

Physical Review Letters 126, 076401 (2021)

186 Reaching the ideal glass in polymer spheres: Thermodynamics and vibrational density of states

Monnier X, Colmenero J, Wolf M, and Cangialosi D.

Physical Review Letters 126, 118004 (2021)

187 Identification of the Mott insulating charge density wave state in 1T-TaS₂

Shin D, Tancogne-Dejean N, Zhang J, Okyay MS, Rubio A, and Park N.

Physical Review Letters 126, 196406 (2021)

188 Phonoritons as hybridized exciton-photon-phonon excitations in a monolayer h-BN optical cavity

Latini S, De Giovannini U, Sie EJ, Gedik N, Hubener H, and Rubio A.

Physical Review Letters 126, 227401 (2021)

189 Light-driven extremely nonlinear bulk photogalvanic currents

Neufeld O, Tancogne-Dejean N, De Giovannini U, Hubener H, and Rubio A.

Physical Review Letters 127, 126601 (2021)

190 Nematicity arising from a chiral superconducting ground state in magic-angle twisted bilayer graphene under in-plane magnetic fields

Yu T, Kennes DM, Rubio A, and Sentef MA.

Physical Review Letters 127, 127001 (2021)

191 Coexistence of superconductivity and spin-splitting fields in superconductor/ferromagnetic insulator bilayers of arbitrary thickness

Hijano A, Ilic S, Rouco M, Gonzalez-Orellana C, Ilyn M, Rogero C, Virtanen P, Heikkila TT, Khorshidian S, Spies M, Ligato N, Giazotto F, Strambini E, and Bergeret FS.

Physical Review Research 3, 023131 (2021)

192 Cubic Hall viscosity in three-dimensional topological semimetals

Robredo I, Rao P, De Juan F, Bergara A, Manes JL, Cortijo A, Vergniory MG, and Bradlyn B.

Physical Review Research 3, L032068

193 The structure of defects, the electron energy-band structure, and the semiconductor-metal transition in PrBaCo₂O_{5.5} cobaltite: Ab initio PAW approach

Zhukov VP, and Chulkov EV.

Physics of the Solid State 63, 395 (2021)

PUBLICATIONS

194 Glass transition and aging of the rigid amorphous fraction in polymorphic poly(butene-1)

Wang W, Fenni SE, Ma Z, Righetti MC, Cangialosi D, Di Lorenzo ML, and Cavallo D.
Polymers 226, 123830 (2021)

195 Modeling ultrasound-induced molecular weight decrease of polymers with multiple scissile azo-mechanophores

Ayer MA, Verde-Sesto E, Liu CH, Weder C, Lattuada M, and Simon YC.
Polymer Chemistry 12, 4093 (2021)

196 Collective motions and mechanical response of a bulk of single-chain nano-particles synthesized by click-chemistry

Maiz J, Verde-Sesto E, Asenjo-Sanz I, Fouquet P, Porcar L, Pomposo JA, De Molina PM, Arbe A, and Colmenero J.
Polymers 13, 50 (2021)

197 Dynamics & spectroscopy with neutrons-recent developments & emerging opportunities

Druzicki K, Gaboardi M, and Fernandez-Alonso F.
Polymers 13, 1440 (2021)

198 Dynamic processes and mechanisms involved in relaxations of single-chain nano-particle melts

Maiz J, Verde-Sesto E, Asenjo-Sanz I, De Molina PM, Frick B, Pomposo JA, Arbe A, and Colmenero J.
Polymers 13, 2316 (2021)

199 Phase transitions in poly(vinylidene fluoride)/polymethylene-based diblock copolymers and blends

Maria N, Maiz J, Martinez-Tong DE, Alegria A, Algarni F, Zapzas G, Hadjichristidis N, and Muller AJ.
Polymers 13, 2442 (2021)

200 Advances in the multi-orthogonal folding of single polymer chains into single-chain nanoparticles

Blazquez-Martin A, Verde-Sesto E, Moreno AJ, Arbe A, Colmenero J, and Pomposo JA.
Polymers 13, 293 (2021)

201 Lignin-stabilized doxorubicin microemulsions: Synthesis, physical characterization, and in vitro assessments

Rahdar A, Sargazi S, Barani M, Shahraki S, Sabir F, and Aboudzadeh MA.
Polymers 13, 641 (2021)

202 Disentangling self-atomic motions in polyisobutylene by molecular dynamics simulations

Khairy Y, Alvarez F, Arbe A, and Colmenero J.
Polymers 13, 670 (2021)

203 Physical aging behavior of a glassy polyether

Monnier X, Marina S, De Pariza XL, Sardon H, Martin J, and Cangialosi D.
Polymers 13, 954 (2021)

PUBLICATIONS

204 Nanoparticle-doped hybrid polyelectrolyte microcapsules with controlled photoluminescence for potential bioimaging applications

Nifontova G, Krivenkov V, Zvaigzne M, Efimov A, Korostylev E, Zarubin S, Karaulov A, Nabiev I, and Sukhanova A. *Polymers* 13, 4076 (2021)

205 Onco-receptors targeting in lung cancer via application of surface-modified and hybrid nanoparticles: A cross-disciplinary review

Sabir F, Qindeel M, Zeeshan M, Ul Ain Q, Randar A, Barani M, Gonzalez E, and Aboudzadeh MA. *Processes* 9, 621 (2021)

206 Mesoscale morphologies of nafion-based blend membranes by dissipative particle dynamics

Sen U, Ozdemir M, Erkartal M, Kaya AM, Manda AA, Oveisi AR, Aboudzadeh MA, and Tokumasu T. *Processes* 9, 984 (2021)

207 A theoretical review on the single-impurity electron spin resonance on surfaces

Delgado F, and Lorente N. *Progress in Surface Science* 96, 100625 (2021)

208 Do calmodulin binding IQ motifs have built-in capping domains?

Muguruza-Montero A, Ramis R, Nunez E, Ballesteros OR, Ibarluzea MG, Araujo A, M-Alicante S, Urrutia J, Leonardo A, Bergara A, and Villarroel A. *Protein Science* 30, 2029 (2021)

209 Frequency-resolved photon correlations in cavity optomechanics

Schmidt MK, Esteban R, Giedke G, Aizpurua J, and Gonzalez-Tudela A. *Quantum Science and Technology* 6, 034005 (2021)

210 External control of qubit-photon interaction and multi-qubit reset in a dissipative quantum network

Zhang XP, Shen LT, Zhang Y, Sun LY, Wu HZ, Yang ZB, and Yin ZQ. *Science China-Physics Mechanics & Astronomy* 64, 250311 (2021)

211 Evidence for a spin acoustic surface plasmon from inelastic atom scattering

Benedek G, Bernasconi M, Campi D, Silkin IV, Chernov IP, Silkin VM, Chulkov EV, Echenique PM, Toennies JP, Anemone G, Al Taleb A, Miranda R, and Farias D. *Scientific Reports* 11, 1506 (2021)

212 a b c d e

Sanroman-Iglesias M, Garrido V, Gil-Ramirez Y, Aizpurua J, Grzelczak M, and Grillo MJ. *Sensors and Actuators B- Chemical* 349, 130780 (2021)

213 High magnetization FeCo nanoparticles for magnetorheological fluids with enhanced response

Vadillo V, Gomez A, Berasategi J, Gutierrez J, Insausti M, De Muro IG, Garitaonandia JS, Arbe A, Iturrospe A, Bou-Ali MM, and Barandiaran JM. *Soft Matter* 17, 840 (2021)

PUBLICATIONS

214 Crowded solutions of single-chain nanoparticles under shear flow

Formanek M, and Moreno AJ.
Soft Matter 17, 2223 (2021)

215 Gold nanoparticles endowed with low-temperature colloidal stability by cyclic polyethylene glycol in ethanol

Aboudzadeh MA, Kruse J, Iglesias MS, Cangialosi D, Alegria A, Grzelczak M, and Barroso-Bujans F.
Soft Matter 17, 7792 (2021)

216 Paper sensors based on fluorescence changes of carbon nanodots for optical detection of nanomaterials

Papadopoulou EL, Biffi G, Senthamizhan A, Martin-Garcia B, Carzino R, Krahne R, and Athanassiou A.
Sustainability 13, 11896 (2021)

PATENTS APPLIED FOR

Apparatus and method for superconducting diode

PCT/IT21/000038

Francesco Giazotto, Elia Strambini, Maria Spiess, Tero Heikkilä, Pauli Virtanen, Stefan Ilic and F. Sebastián Bergeret Sbarbaro.

Low temperature production of synthetic wollastonite

21306331

Valentina Musumeci, Cyril Aymonier, and Jorge Sánchez Dolado.

Method for colorimetric detection of bacteria in food samples

PCT/EP21/068470

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

EDUCATION



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. In the following we note the main aspects of the training activities at CFM.

POST-DOCTORAL TRAINING

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

PHD PROGRAM: PHYSICS OF NANOSTRUCTURES AND ADVANCED MATERIALS

“Physics of Nanostructures and Advanced Materials” is a PhD program of UPV/EHU that has been recognized as a highly qualified PhD program by the Spanish Ministry of Education (MEE2011-0591 citation of excellence). Within this program, 70 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

- **Theory of spin-orbit interactions in electronic transport and light scattering at the mesoscale**
Author: Cristina Sanz Fernández
Supervisor: F. Sebastián Bergeret Sbarbaro and Prof. Juan José Sáenz
Group: Mesoscopic Physics
03/02/2021
- **Classical dynamics of gas-surface scattering: fundamentals and applications**
Author: Alberto Rodríguez Fernández
Supervisors: Ricardo Díez Muiño and Laurent Bonnet
Group: Gas/Solid Interfaces
05/02/2021
- **A unifying approximation scheme for density functional theories: A force balance based approach**
Author: Mary-Leena Martine Tchenkoue Djouom
Supervisors: Michael Ruggenthaler and Angel Rubio Secades
Group: Nano-bio Spectroscopy
19/03/2021

- **A supercritical water-based technology for calcium silicate hydrate nanoparticles production**
Author: Valentina Musumeci
Supervisor: Jorge Sánchez Dolado
Group: Ceramic and Cement-based Materials
31/03/2021
- **Theoretical approach to atomic-scale nanoplasmonics as probed by light and swift electrons**
Author: Mattin Urbieto Galarraga
Supervisors: Nerea Zabala Unzalu and Javier Aizpurua Iriazabal
Group: Theory of Nanophotonics
06/05/2021
- **Magnetism at the nanoscale: Electron spin resonance**
Author: José Reina Gálvez
Supervisors: Nicolás Lorente Palacios and Fernando Delgado Acosta
Group: Quantum Phenomena on Surfaces
12/05/2021
- **Ab initio strong light-matter theoretical framework for phenomena in non-relativistic quantum electrodynamics**
Author: Davis Dave M. Welakuh
Supervisors: Angel Rubio Secades and Michael Ruggenthaler
Group: Nano-bio Spectroscopy
08/06/2021
- **Modelling light-induced charge-transfer from transition-metal-doped aluminium clusters to carbon dioxide**
Author: Alexandra Göbel
Supervisors: Angel Rubio Secades and Johannes Lischner
Group: Nano-bio Spectroscopy
20/08/2021
- **Electron scattering and static field effects in high-order harmonic generation in solid systems**
Author: Chang-Ming Wang
Supervisors: Angel Rubio Secades and Nina Rohringer
Group: Nano-bio Spectroscopy
29/09/2021
- **Structure and function in single-chain nanoparticles**
Author: Julen de la Cuesta Leone
Supervisors: José A. Pomposo Alonso
Group: Polymers and Soft Matter
05/11/2021

- **Dynamics and structural features of biomolecules in aqueous environments - The cases of water and ice**
Author: Jorge Humberto Melillo
Supervisors: Silvina Cervený Murcia and Alexander Bittner
Group: Polymers and Soft Matter
 01/12/2021
- **Superconductivity in the presence of Spin-Dependent Fields**
Author: Mikel Roucco
Supervisors: F. Sebastián Bergeret Sbarbaro and Ilya Tokatly
Group: Mesoscopic Physics
 18/11/2021
- **Topological materials from a symmetry perspective**
Author: Iñigo Robredo Magro
Supervisor: Maia García Vergniory and Aitor Bergara Jauregi
Group: Quantum Theory of Materials
 10/12/2021
- **Generation of laser-driven shocks and their use to study simple compounds at high pressure**
Author: Donald Mancelli
Supervisors: Dimitri Batani and Ion Errea Lope
Group: Quantum Theory of Materials
 15/12/2021

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 5 pre-doctoral researchers 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 2021:

- | | |
|--|---|
| <ul style="list-style-type: none"> • Antonella Meninno
 IMPMC of the Sorbonne Université (France)
 12 April – 11 July | <ul style="list-style-type: none"> • Carmen González Orellana
 NEST Istituto Nanoscienze (Italy)
 15 September - 8 December |
| <ul style="list-style-type: none"> • Alba Jumbo Nogales
 University of Bordeaux (France)
 1 September - 31 October | <ul style="list-style-type: none"> • Cristina Mier González
 Center for Quantum Nanoscience, Seoul (Korea)
 9 September - 10 December |
| <ul style="list-style-type: none"> • Balthasar Braunewell
 Elettra Sincrotrone Trieste (Italy)
 1 September – 31 October | |

PHD RECRUITMENT FAIR 2021

In 2021 CFM organized the fourth PhD Recruitment Fair as part of the strategic plan to recruit new talent. From the 136 applications received, 26 applicants were shortlisted 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:

- **Alaa Mohammed Idris Bakhit**
Group: Nanophysics Lab
Supervisor: Frederik Michael Schiller
- **Malen Etxeberria Etxaniz**
Group: Modelisation and Simulation
Supervisor: Andrés Arnau Pino
- **Francesco Coin**
Group: Polymers and Soft Matter
Supervisor: Silvina Cervený
- **Paula Angulo Portugal**
Group: Nanophysics Lab
Supervisor: Martina Corso
- **Ivan Žugec**
Group: Gas/Solid Interfaces
Supervisor: Iñaki Juaristi Oliden
- **Zuzanna Lawera**
Group: Nanomaterials and Spectroscopy
Supervisor: Marek Grzelczak
- **Jon Ortuzar Andrés**
Group: Mesoscopic Physics
Supervisor: F. Sebastián Bergeret Sbarbaro



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.

SCHOLARSHIPS

The Materials Physics Center (MPC) research association offers scholarships to highly motivated graduates who are planning to complete their studies with a Master's degree.

In 2021, five graduates were awarded scholarships for the Master in Nanoscience program:

- **Paula Angulo Portugal**
Supervisors: Martina Corso and Jose Ignacio Pascual
- **Divya Jyoti**
Supervisors: Nicolás Lorente Palacios and Deungjang Choi
- **Francisco Romero Lara**
Supervisors: Martina Corso and Thomas Frederiksen
- **Ebtisam Tarek**
Supervisor: Maider Ormaza Saezmiera and Enrique Ortega Conejero
- **Malen Etxeberria Etxaniz**
Supervisors: Aitor Bergara Jauregi and Aritz Leonardo Liceranzu

THESES OF THE NANOSCIENCE MASTER SUCCESSFULLY DEFENDED IN 2021

- **Magnetic materials characterization using magneto ellipsometry approaches**
Author: Carmen Martín Valderrama
Supervisor: Andreas Berger
- **Membranes for ammonia synthesis**
Author: Noelia Sánchez Ortega
Supervisor: Margot Llosa Tanco
- **Superconductivity in MoS₂ intercalated with organic molecules**
Author: Yaiza Asensio García
Supervisors: Luis Hueso Arroyo and Marco Gobbi
- **Growth of Boron Nitride by atomic layer deposition**
Author: Ana Álvarez Yenes
Supervisors: Victor Koroteev and Mato Knez
- **Growth and electronic structure of two-dimensional transition metal dichalcogenide in-plane heterostructures**
Author: Paula Angulo Portugal
Supervisors: Martina Corso and Jose Ignacio Pascual
- **Superconducting gap engineering**
Author: Divya Jyoti
Supervisors: Nicolás Lorente Palacios and Deungjang Choi
- **Synthesis of cyclic and linear branched polyglycidols**
Author: Mohammed Ali Al Assiri
Supervisor: Fabienne Barroso Bujans
- **Chiral induced spin polarization in elemental Tellurium**
Author: Manuel Suárez Rodríguez
Supervisors: Fèlix Casanova i Fernàndez and Beatriz Martín García
- **Au thin films on Si prepatterned substrates for plasmonic applications**
Author: Kevin García Díez
Supervisors: Enrique Ortega Conejero and Andrew Weber
- **Emergence of magnetism in open-shell graphene nanostructures**
Author: Francisco Romero Lara
Supervisors: Martina Corso and Thomas Frederiksen
- **Growth and characterization of ZnO on a curved Cu crystal**
Author: Ebtisam Tarek
Supervisors: Maider Ormaza Saezmiera and Enrique Ortega Conejero

- **Active tuning of phonon polaritons in twisted Van der Waals heterostructures**
Author: Arturo González Morán
Supervisors: Alexey Nikitin and Pablo Alonso González
- **Coupling RF to a superconducting STM Junction**
Author: Alfonso García Gómez
Supervisor: José Ignacio Pascual
- **Molecular dynamics study of calmodulin in Kv7.2 channels**
Author: Malen Etxeberria Etxaniz
Supervisors: Aitor Bergara Jauregi and Aritz Leonardo Liceranzu
- **Data-driven prediction of nanoparticle geometry in real-time**
Author: Xabier Belaunzaran Sanz
Supervisor: Marek Grzelczak
- **Synthesis and characterization of nanoparticles for temperature sensing**
Author: Miriam Martínez Flórez
Supervisors: Carlos Renero Lecuna and Luis Liz Marzán
- **Spectral and spin-dependent properties of superconducting systems with Yu-Shiba-Rusinov states**
Author: Jon Ortuzar Andrés
Supervisors: José Ignacio Pascual and F. Sebastián Bergeret Sbarbaro
- **Single-chain nanoparticles via metal-free click-chemistry: Synthesis and characterization**
Author: Ana-Maria Stan
Supervisors: Jose A. Pomposo Alonso and María Ester Verde Sesto



OTHER MASTER THESES PROJECTS SUPERVISED BY CFM STAFF AND SUCCESSFULLY DEFENDED IN 2021

- **Invecchiamento fisico della frazione amorfa rigida nel polietilenossido**
Author: Claudio Magnani (Geneve University)
Supervisor: Daniele Cangialosi
- **Theoretical study of hBN ribbon resonances induced by a near-field probe**
Author: Elise Prin (Bordeaux University)
Supervisor: Javier Aizpurua Iriazabal

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. After the restrictions caused by the general sanitary emergency, this program was fully recovered in 2021. CFM hosted the visit of 12 undergraduate students. Among them, the following eight fulfilled and defended their end of course projects:

- **Structure and chemical properties of CeO₂ on a curved Cu(111) crystal**
Author: Lorena Glatthaar (JLU Giessen)
Supervisor: Frederik Schiller
- **Fotosintesi artificiale burutzeko material hibrido berriak**
Author: Aimar Marauri Iriberrri
Supervisor: Marek Grzelczak and Jon Mattin Matxain Beraza
- **Computational analysis of 12 mutations in the potassium channel KCNQ2**
Author: Amaia Razquin Lizarraga
Supervisors: Aitor Bergara Jauregi and Aritz Leonardo Liceranzu

- **Analysis of plasmonic nanostructures using the quasinormal mode formalism**
Author: Xabier Arrieta Aristi
Supervisors: Nerea Zabala Unzalu and Rubén Esteban Llorente
- **Prospección de celulosa bacteriana obtenida en el proceso de elaboración de Kombucha**
Author: Juan Manuel Garzón Vela
Supervisors: Javier Martínez Sabando and Silvina Cervený Murcia
- **Estudio de redes poliméricas basadas en poliglicidol**
Author: Eric Gómez Urreizti
Supervisors: Fabienne Barroso Bujans and Ángel Alegría Loinaz
- **Sistema automatizado para acelerar la optimización de catalizadores nano-estructurados para fotosíntesis artificial**
Author: Joseba Solozabal Aldalur
Supervisor: Marek Grzelczak
- **Nuevas rutas de síntesis de nanopartículas poliméricas unimoleculares**
Author: Aínara Ruiz Bardillo
Supervisor: José A. Pomposo Alonso and Ester Verde Sesto

CFM also offers the possibility to receive support for this training through different grant programs. In 2021, the following 4 students received such grants:

- **Iñaki Fernández Tena**
Supervisor: Maite Alducin Ochoa
- **Aínara Ruiz Bardillo**
Supervisor: José A. Pomposo Alonso
- **Joseba Solozabal Aldalur**
Supervisor: Gabriel Molina Terriza
- **Janire López Campos**
Supervisor: Silvia Arrese-Igor Irigoyen

WORKSHOPS, CONFERENCES AND SEMINARS

The background of the page features a photograph of a conference room. Several people are seated at long wooden tables with red upholstered chairs. They are wearing face masks and appear to be engaged in a meeting. One person in the foreground is using a laptop. Overlaid on the right side of the image is a decorative graphic consisting of numerous teal and blue geometric shapes, including hexagons and elongated rectangles, arranged in a pattern that suggests movement or a network.

CFM has been able to adapt the format of the conferences to the needs of the post-pandemic situation, organizing or co-organizing **10 international workshops and conferences during 2021**.

Many of these meetings are 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 attended requests to give **58 invited and plenary talks** in international conferences, showing their leadership in their respective fields.

The list of conferences, courses, workshops and seminars organized or co-organized by CFM researchers during 2021 is as follows:

CONFERENCES

QENS/WINS 2021 International Conference

Organizers: Arantxa Arbe Mendez (Chair, CFM), and Juan Colmenero de Leon (co-Chair, CFM).

Online

17-21/5/2021

IV International Meeting on Science and Literature

Organizer: Gustavo A. Schwartz Pomeraniec (CFM).

DIPC

22-24/11/2021

Quantum Conference 2021

Organizers: Antonio Correia, Ricardo Díaz Muiño (DIPC and CFM), Pablo Ordejon, Valerio Pruneri, Stephan Roche, and Daniel Sanchez Portal (CFM).

BEC, Barakaldo, Spain

23-25/11/2021

WOKSHOPS

Software Carpentry Online Workshop

Organizers: Iñigo Aldazabal Mensa (CFM), Rohit Goswami, Raphaela Heil, and Sonia Olaechea.

Online

16, 17, 23 and 24/03/2021

Faraday Conference

Organizers: RSC Faraday Division (Felix Fernández Alonso, CFM).

Online

29-31/3/2021

QNS-DIPC joint online workshop on Quantum Control and Quantum Technologies

Organizers: Deungjang Choi (CFM), Nicolás Lorente Palacios (CFM), Ricardo Díez Muiño (CFM, DIPC), and Andreas Heinrich.

Online

8-9/6/2021

International Dielectric Society

Organizers: Ranko Richert, Catalin Gainaru and Silvina Cervený Murcia (CFM).

Online

6-9/9/2021

Challenges in reaction dynamics of gas-surface interactions and methodological advances in dissipative and nonadiabatic processes (CECAM workshop)

Organizers: Maite Alducin Ochoa (CFM), Didier Lemoine, Rocco Martinazzo, Peter Saalfrank, and Jean Christophe Tremblay.

Grand Hôtel d'Orléans, Toulouse, France

27-30/9/2021

RSC Statistical Mechanics and Thermodynamics Group Early Career Symposium

Organizers: Fernando Bresme, and Félix Fernández Alonso (CFM).

Online

17/11/2021

RSC Statistical Mechanics and Thermodynamics Group

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

Online

2021- On going



COURSES

La ciencia de los jinetes del apocalipsis: Una aproximación científica a los riesgos existenciales de la humanidad

Organizers: Juan Ignacio Pérez Iglesias, and Ricardo Díez Muiño (DIPC, CFM).

Miramar Palace, Donostia / San Sebastián

12-14/07/2021

Learning the basics with insights (DIPC Courses)

Organizers: Deungjang Choi (CFM, DIPC), and Nicolás Lorente Palacios (CFM, DIPC)

DIPC and online

2021- On going

SEMINARS ORGANIZED BY CFM

Gender Equality and Diversity at CFM: State of the art and harassment protocol

Daniel Sánchez Portal (CFM) and Idoia Mugica Mendiola (CFM)

Online

2/6/2021

Towards a predictive ab initio theory for nonlinear transport phenomena

Stepan Tsirkin (Physik Institut-Condensed Matter Theory, University of Zurich)

CFM Auditorium

25/6/2021

TRANSFERABLE SKILLS PROGRAM

Equipping researchers with skills beyond the purely scientific is a challenge that institutions are beginning to take up in the framework of what is known as the "transferable skills" education programs. Organized by Aitzol García Etxarri (DIPC) and Gustavo A. Schwartz Pomeranec (CFM), DIPC and CFM have launched a full program covering issues like stress management, media training or transformative leaderships. More than 200 researchers joined these courses in 2021.

Stress Management

Sofia Facal and Manuela Bercioux
(Skills4Science)

CFM auditorium

3-4/2/2021

Stress is a normal physical reaction and can be positive in short bursts, but over long periods of increased stress exposure, it leads to a decrease in personal wellbeing and work efficiency. A worldwide PhD survey conducted by Nature in 2019 reported a high level of stress connected problems within PhD students. This has drawn attention to an increasing problem that is affecting many researchers. The COVID-19 pandemic has further intensified the problem, highlighting the need to develop a program to give practical strategies to prevent and manage stressful situations. With this workshop CFM and DIPC aim to support their researchers, especially at the early stage of their careers, by offering the tools to recognize the stress signals and learn how to cope with them.

Transformative leadership

Sofia Facal and Manuela Bercioux
(Skills4Science)

CFM auditorium

13-15/9//2021

Oriented to Senior Scientists (including those just starting their scientific careers), this workshop explored transformational leadership skills in research and academia. In contrast to traditional leadership styles, transformational leadership is focused on encouraging, inspiring, and motivating colleagues and young researchers to innovate and create change, take responsibility and reach performance beyond expectations.

Providing leadership education can be a way to extend a science graduates' outlook, capacity, and employability. It can constitute a pathway for building self-awareness, self-efficacy, interpersonal skills, resilience, and adaptability, all transferable skills employers seek.

Media Training

Valentina Rodríguez

DIPC

6/5/2021

The workshop aimed to help our researchers improve their communication abilities in the context of media interviews. The participants learned how and why some scientific stories become a piece of important news. The idea was to help the attendants to identify personal strategies and abilities that will let them communicate their scientific work in a more effective way in media interviews.

This course was conducted by Valentina Rodríguez, a science communication professional with extensive experience in science journalism and astronomy outreach for international observatories.

Consejos a un/a joven científico/a

Pedro Miguel Echenique
Landiribar

1-2/12/2021

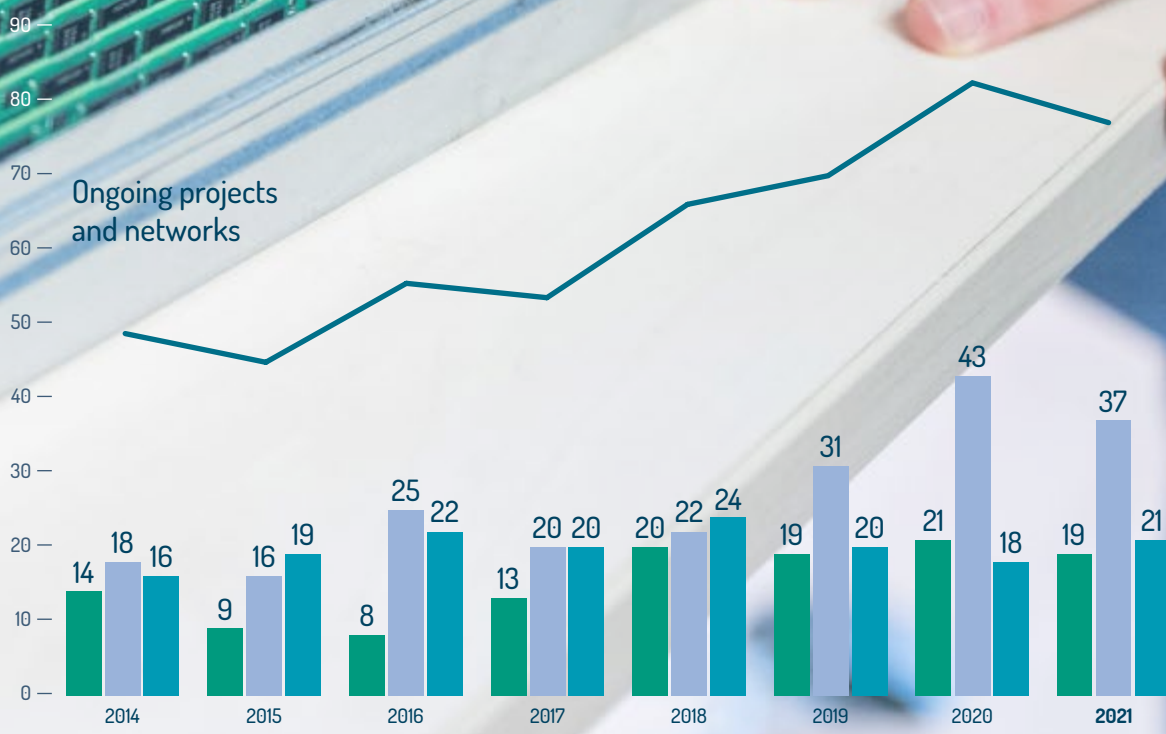
DIPC

In this talk, Professor Pedro Miguel Echenique, president of the Donostia International Physics Center (DIPC) and researcher at CFM, discussed on the training stage of young scientists, giving advice and guidance. The talk, full of content of undoubted interest, was recommended to all the people who are studying their doctorate in our scientific community.



COMPETITIVE FUNDING FOR RESEARCH PROJECTS

RESEARCH PROJECTS AND NETWORKS	Competitive public fundraising in 2021
■ BASQUE	565.335,46 €
■ SPANISH	1.219.495,00 €
■ INTERNATIONAL	2.121.614,96 €
MPC-BERC	1.224.640,00 €
— TOTAL	5.131.085,42 €



The projects and networks ongoing during 2021 (a total of 77 projects/networks) are listed below according to the source of competitive funding.

BASQUE RESEARCH PROJECTS AND NETWORKS

- **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, 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, and Aitor Bergara Jauregui
- **EJ/GV, Proyectos de Investigación Básica y/o Aplicada 2021-2023 (PIBA), PIBA2021_1_0026**
Propiedades estructurales y electrónicas de perovskitas híbridas en condiciones variables de presión, temperatura, interfaces e iluminación
PI: Lucia Vitali

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- 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
 - 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
 - Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa Coopera 2020, 2020-IZEN-000012-01**

ELLAS INVESTIGAN VI: Afrikan emakumezko ikertzaile batek egonaldi bat egin dezan MPCn / ELLAS INVESTIGAN VI: 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: Afrikan 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, SAREA2021 RED2021, Mod. Equipamiento, 2021-CIEN-000032-01**

Adquisición de un sistema de análisis químico basado en espectroscopia electrónica Auger

PI: Lucia Vitali
 - Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2021 RED2021, Mod. Gipuzkoa NEXT, 2021-CIEN-000107-01**

Luz y diamantes: Computación cuántica en Donostia

PI: Gabriel Molina Terriza

BASQUE RESEARCH PROJECTS AND NETWORKS

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2021 RED2021, Mod. Proyectos I+D, 2021-CIEN-000010-01**

Desarrollo de nanomateriales quimio-luminiscentes con aplicación en la detección de enfermedades inflamatorias graves

PI: Josetxo Pomposo Alonso

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2020 RED2020, Mod. Proyectos I+D, 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, EHUKo Sailentzako Laguntzak/Ayudas Departamentos UPV 2020, DEP20/61**
Polímeros y materiales avanzados: Física, química y tecnología

PI: Iñaki Juaristi Oliden

- **UPV/EHU, INT-EHUrOPE 2019, EHUrOPE19/01**
From water to oxygen and vice versa: Correlating structure, activity and selectivity of a model bifunctional catalyst

PI: Sara Barja Martínez



SPANISH RESEARCH PROJECTS AND NETWORKS

- **Proyectos en Líneas Estratégicas 2021, colaboración público-privada (PLEC2021), PLEC2021-008251**

Few-qubit quantum hardware, algorithms and codes, on photonic and solid-state systems

PI: Gabriel Molina Terriza

- **Proyectos de I+D+i de Generación de Conocimiento 2020 (PID2020), PID2020-114506GB-I00**

HYPER – Facing the hybrid-perovskite challenge – new insights into the stability, degradation and performance of next-generation photovoltaic & photonic materials

PI: Félix Fernández Alonso

- **Proyectos de I+D+i de Generación de Conocimiento 2020 (PID2020), PID2020-114252GB-I00**

SPIRIT – Spintronics and Spin-orbitronics in Hybrid Nanostructures: From classical to Quantum Technologies

PI: Sebastián Bergeret Sbarbaro

co-PI: Vitaly Golovach

- **Proyectos de I+D+i de Generación de Conocimiento 2020 (PID2020), PID2020-115419GB-C22**

Vidrios y vitrocerámicos nanoestructurados dopados con tierras raras para aplicaciones fotónicas (subproyecto)

Proyecto coordinado: LUMGLASS – Processing and photonic applications of luminescent glasses and glass-ceramics

PI: Rolindes Balda de la Cruz

- **Proyectos de I+D+i de Retos Investigación 2020 (PID2020), PID2020-116093RB-C44**

MODCAT – Unveiling structure-function relationships on model catalyst for the clean generation of high added value chemical products (subproyecto)

Proyecto Coordinado: ECOCAT – Electrocatalysis for the sustainable production of fuels and high added-value chemicals

PI: Sara Barja Martínez

Co-PI: Frederik Michael Schiller

SPANISH RESEARCH PROJECTS AND NETWORKS

- **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**
Revers02 – Oxygen conversion reactions: Fundamental insights for rational design
PI: 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 Cervený 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 Muño
- **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

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- **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 fotocatalisis 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)
 - **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
 - **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

SPANISH RESEARCH PROJECTS AND NETWORKS

- **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**
OSMoISis – 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 I+D Fundamental (Excelencia) 2017, FIS2017-87363-P**
Nanofotónica cuántica: Explorando las correlaciones cuánticas de los fotones usando nanopartículas
PI: Gabriel Molina Terriza
- **Proyectos I+D Fundamental (Excelencia) 2017, MAT2017-87035-C2-2-P**
Vidrios y vitrocerámicos dopados con tierras raras para aplicaciones fotónicas
PI: Rolindes Balda de la Cruz

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- **Retos Investigación 2017, MAT2017-88377-C2-2-R**
Transistores de spin basados en heteroestructuras Van der Waals
PI: Sara Barja Martínez
co-PI: Miguel Moreno Ugeda (DIPC, Ikerbasque)
 - **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
 - **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
 - **Proyectos I+D Fundamental (Excelencia) 2016, FIS2016-77188-P**
Teoría y simulación de fenómenos ópticos y de transporte en materiales girotrópicos
PI: Ivo Souza
 - **CSIC, I-COOP+ 2020, Cooperación Científica para el Desarrollo, COOPB20502**
Arsenic-free, new nano-structured multifunctional materials to remove arsenic in groundwater
PI: Silvina Cervený Murcia
 - **CSIC, I-LINK+ 2019, Colaboración Científica Internacional, LINKC20002**
On-surface polymerization for high performance (opto)electronics
PI: Martina Corso

SPANISH RESEARCH PROJECTS AND NETWORKS

- **CSIC, I-COOP+ 2019, Cooperación Científica para el Desarrollo, COOPB20432**
Diluted magnetic quantum dots assemblies for innovative spintronics
PI: Martina Corso
- **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 Cervený Murcia
- **CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2020, 2020AEP178**
Magnetismo exótico y fenómenos de correlación de electrones en la superficie y el sólido de materiales basadas en tierras raras
PI: Frederik Michael Schiller
- **CSIC, Fondo de Apoyo a los Servicios Científico-Técnicos (FAS) 2020, FAS2020_058**
Unidad de control 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 Synergy Grant (ERC-2020-SyG), GA 951281**
BOLD - A background-free experiment to discover the nature of neutrinos based on single Barium Atom Light Detection
PI: Celia Rogero Blanco
- **ERC Starting Grant (ERC-2020-StG), GA 946629**
PhotoNow - Discovery and characterization of third-generation nonlinear photovoltaics
PI: Julen Ibañez Azpiroz
- **ERC Starting Grant (ERC-2018-StG), GA 802533**
SuperH - Discovery and characterization of hydrogen-based high-temperature superconductors
PI: Ion Errea Lope
- **ERC Advanced Grant (ERC-2015-AdG), GA 694097**
QSpec-NewMat - Quantum Spectroscopy: Exploring new states of matter out of equilibrium
PI: Ángel Rubio Secades
- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN-01-2018-2019-2020), GA 964450**
MIRACLE - Photonic Metaconcrete with Infrared RAdiative Cooling capacity for Large Energy savings
PI: Jorge Sánchez Dolado
- **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

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

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

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- **INFRAIA: Integrating Activities for Advanced Communities (H2020 INFRAIA-2016-1), GA 731019**
EUSMI – European infrastructure for spectroscopy, scattering and imaging of soft matter
PI: Ángel Alegría Loinaz
 - **Marie Curie Individual Fellowship (H2020-MSCA-IF-2020), GA 101030868**
MAGNIFI-Nuclear Magnetic resonance augmented by Nitrogen-vacancy centres and Field versatility
Supervisor: Gabriel Molina Terriza
 - **Marie Curie Individual Fellowship (H2020-MSCA-IF-2020), GA 101025664**
QESPEM: Light-controlled bright and stable plexcitonic quantum emitters operating in both single-photon and entangled photon-pair emission modes
Supervisor: Yury Rakovich
 - **Marie Curie Individual Fellowship (H2020-MSCA-IF-2018), GA 839237**
PhotoWann – Bulk Photovoltaic effect via Wannier functions
Supervisor: Ivo Souza
 - **COST Action 2017, CA17139**
EUTOPIA – European Topology Interdisciplinary Action
Management Committee Member: Ángel Moreno Segurado
 - **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 Cervený Murcia
 - **INTERREG (ETC) V A: Cross-border Cooperation, POCTEFA 2014-2020, EFA194/16/TNSI**
TNSI-Trans-Pyrenean Node for Scientific Instrumentation
PI: Celia Rogero Blanco
 - **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

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 2021. 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 cementárň (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 (VI 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 European Industrial Network (see Research Funding Section).

SCIENCE AND SO

At CFM, supporting scientific culture is a core policy in our understanding of the scientific community's duty to society. The year 2021 has been a year of settling into the new forms of communication that the global pandemic situation required us to adopt. It is worth mentioning that the way we address society has necessarily changed. While adapting to the new dynamics supposed a great effort, CFM has been able to continue to offer a complete program that guarantees a direct relationship with society, recovering spaces and reinventing activities.

During 2021 more than 60 activities and events were organized, many of them in collaboration with other institutions.

More than 9000 people were able to participate in the activities organized despite the limitations for social relations. Thanks to all the attendees.



CIETY



More than 40 researchers of CFM's staff participated in the outreach program of the center. Thanks to all of them.

Culture, Vocation, and Gender perspective: We do care

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

SCHOOL VISITS

Starting in 2013, together with the Donostia International Physics Center (DIPC), CFM offered a program of visits where both centers opened their doors to high school students.

Given the impossibility of continuing with the face-to-face format, in 2021 we launched a program of online visits that has become a huge success, reaching more than **700 students** that were able to interact with more than **20 professionals** of DIPC and CFM.

In each visit the schools have the chance to video chat directly with our researchers as well as virtually visit the following premises thanks to a set of **videos** professionally recorded for this purpose:

- **Calculus Center of DIPC**
- **Polymer synthesis lab at CFM**
- **Dielectric spectroscopy lab at CFM**
- **Nanophysics lab at CFM**



Available at **CFM's YouTube channel** or scanning this code

EMAKUMEAK ZIENTZIAN 2021

emakumeakzientzian.eus

8-28/02/2021

CIC nanoGUNE, CIC biomaGUNE, DIPC, Biodonostia, Polymat, Elhuyar, CEIT, TECNUN, Eureka! Zientzia Museoa, the Faculty of Informatics (UPV/EHU) and CFM

SCIENCE IS INDEED A GIRLS' THING

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, the Emakumeak Zientzian initiative was borne, to unite the forces of different research centers and science institutions of the Donostia / San Sebastian area, to make visible the activity of women in science, to break with the typically masculine roles attributed to scientific-technical activities, and to encourage the choice of scientific careers among girls and adolescents.

In 2021, on its 5th edition, DIPC and CFM co-ordinated the full program that brought together the activities of **11 research centers and science-related institutions**.



In addition to the commitment of the different entities, the initiative has achieved the support of the Provincial Council of Gipuzkoa, CSIC, the FECyT and Fomento San Sebastián, which have sponsored the event with different financial contributions.

#EmakumeakZientzian presented a full program that aimed at all the public, specially focusing on teenager women, school kids, elder women (above 55), and also the scientific community.

It is worth mentioning that in this edition, 15 activities were organized and 21 **videos of public events**, experiments, and virtual visits were produced as a complement to the limited face-to-face activities.



Available at
#EmakumeakZientzian
YouTube channel or
scanning this code

2410

Direct Participants
(face to face and streaming)

2920

Visualizations

30

Impacts in Media

11

Entities

15

Activities

+ 40

Volunteers involved



“QUÉ SABEMOS DE...” TALK SERIES

KUTXAKULTUR PLAZA AT TABAKALERA, DONOSTIA / SAN SEBASTIÁN

5, 12, 19 and 26/11/2021

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.



Available at **CFM's YouTube channel** or scanning this code

- **Exoesqueletos: Robótica y automática**

Elena García Armada

CEO in Marsi Bionics and CSIC Researcher



- **El agua es rara**

Silvina Cerveny Murcia

CSIC Researcher at the Polymers and Soft Matter group at CFM



- **Patologías causadas por el SARS-CoV-2 y estrategias de protección frente al virus**

Luis Enjuanes Sánchez

Research Professor and Head of the Coronavirus Laboratory at the National Biotechnology Centre of the CSIC



- **Desmontando mitos alimentarios a conciencia**

Miguel Herrero Calleja

Research Scientist at the Instituto de Investigación en Ciencias de la Alimentación (CIAL) of the CSIC



XVI SCIENCE WEEK (UPV/EHU)

Tabakalera, Donostia / San Sebastián

5-7/11/2021

From the 5th to the 7th of November 2021, CFM together with DIPC and CIC nanoGUNE, joined the UPV/EHU's science week that every year gathers thousands of visitors to enjoy the full program of activities devoted to all public.

- **Scale up your world**

Tailor designed workshop on the world of scales, from macro to nano, devoted to families.

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

- **Zientzia Kluba**

Humor and a lot of science were the components of the Zientzia Kluba formula. At this show organized by UPV/EHU, monologues, talks, performances, or the perfect mix of it all were welcome.

In 2021, CFM researcher Gabriel Molina Terriza participated with the following talk:

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

- **The Game of Brainy Roles**

In this workshop devoted to school teachers, José A. Martínez González, researcher at CFM's Polymers and Soft Matter group, and his colleague Maria Larriba Hormigos, presented and showed how to use a game of their creation: The Game of Brainy Roles. The game is based on collaboration and role-playing, where players have to work in groups to develop a multidisciplinary research project that will allow them to approach a research challenge in the most creative way possible by following the scientific method.

PRIDE IN STEAM DAY


orgulloenciencia.dipc.org

18/11/2021

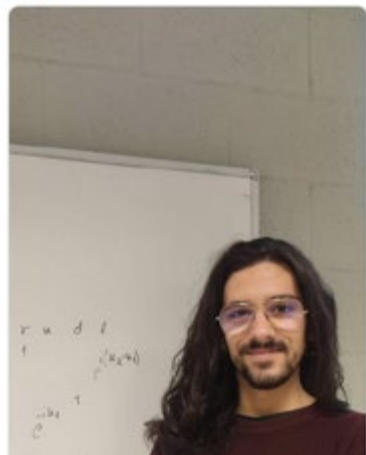
In 2019 the DIPC, CIC nanoGUNE and CFM created the space "Pride in Science- Donostia" to send a message loud and clear: in science the more diverse, the better. Breaking stereotypes is vital, and to that end, giving visibility to scientists of the LGTBQIA+ collective is fundamental to create new references.

In 2021, we organized a campaign in our social media. The aim of the campaign was to present our centers as a safe space to work in, maximizing the visibility of the researchers and staff of DIPC, CIC nanoGUNE and CFM that belong in the LGTBQIA+ community.

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

 **CFM**
@CFMdonostia

I'm [@ma_jherrer](#), predoc researcher in theoretical physics, and a openly gay man. My work is focused on the topological characterization of the different phases two-dimensional electronic lattices can display. It is vital not to feel ashamed about your identity
[#quantum](#)
Thanks! Tere



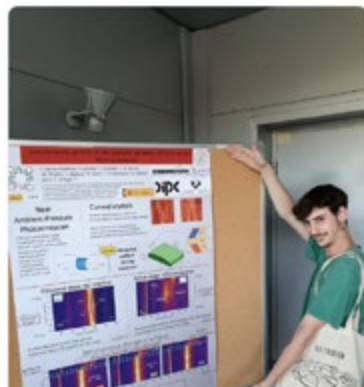
 **CFM**
@CFMdonostia

I'm [@garciaetxarri](#). I'm a queer researcher at [@DIPC](#), where I lead a research group on [#nanophotonics](#). We study light-matter interactions in the nanoscale and find applications in neuroscience, topology photonics and separation of chiral molecules.
[#HarotasunaZientzia](#)
Thanks! Tere



 **CFM**
@CFMdonostia

I am Fernando Garcia Martinez, a gay Predoc researcher at [@CFMdonostia](#). I work on Surface Chemistry (how the surface of some catalysts behave under reaction conditions, and how this influences the turnover of the reaction). Science should be a place for equality and diversity
Thanks! Tere



 **CFM**
@CFMdonostia

[@idolamugka](#), outreach manager and coordinator of the [#GenderEqualityPlan](#) at [@CFMdonostia](#). Dr in organic chem working full time on [#scicomm](#), trying to bring science and society closer, with [#genderequality](#) and [#diversity](#) perspective from CFM. [Bisexual](#) and mother
Thanks! Tere



 **CFM**
@CFMdonostia

I'm Marina Peña-Díaz, Predoc researcher in the [@nanophyslab](#) of [@CFMdonostia](#). I work on the study of basic problems of electrocatalysis of fuel cell reactions, focusing on metal-oxides for the oxygen evolution reaction (OER). [#Renewable energy](#) [#Xray](#) [#STM](#)
Thanks! Tere



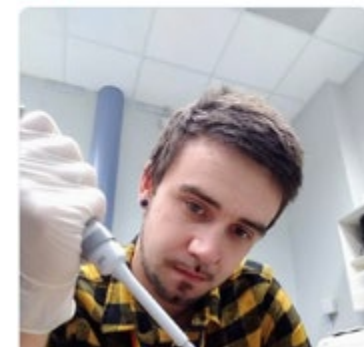
 **CFM**
@CFMdonostia

I'm Matteo Zennaro and I'm a gay postdoc researcher at [@DIPCehu](#)! My field of research is [#cosmology](#) and I study, through computer simulations, what our Universe is made of, and look for the lightest particle neutrino's mass by analysing galaxies distribution.
Thanks! Tere



 **CFM**
@CFMdonostia

I'm Stephen O'Brien, a postdoctoral researcher currently working in the Nanoengineering Group of [@nanoGUNE](#). My current research focuses on the use of machine learning assisted vibrational spectroscopy for the detection and diagnosis of a range of illnesses.
Thanks! Tere



FOTCIENCIA

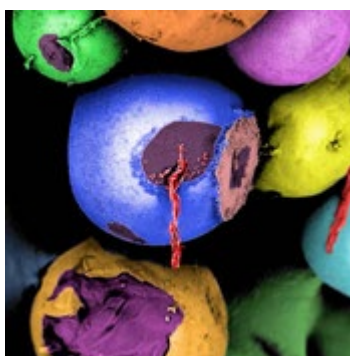
Eureka! Zientzia museoa,
Donostia / San Sebastián

02/12/2020 - 17/01/2021

FOTCIENCIA is a photography contest organized yearly by Consejo Superior de Investigaciones Científicas (CSIC) and Fundación Española para la Ciencia y la Tecnología (FECYT) in collaboration with Jesús Serra foundation. The aim of the initiative is to bring science closer to the society inviting researchers as well as citizens to participate in two categories: macro and microscopic photography.

As a result of the contest, a photo exhibit is yearly launched. This exhibit travelled more than 20 cities in 2021, and CFM in collaboration with Eureka! Zientzia Museoa had the pleasure to host it in Donostia / San Sebastián, continuing with the tradition implemented for the last four years.

More than 1 900 attendees visited the exhibit.



“A LIFE IN SCIENCE” IN EUREKA! ZIENTZIA MUSEOA

Eureka! Zientzia Museoa, Donostia / San Sebastián

25/10/2021 and 8/11/2021

Since 2010, Eureka! Zientzia Museoa (the science museum in Donostia / San Sebastián) organizes a meeting that resembles the format of a scientific congress, where active professionals of different scientific disciplines present their “life in science” to high school students with poster sessions and oral contributions. It is a great opportunity for both researchers and students to meet and share experiences and inquiries.

CFM supports this successful initiative by sponsoring the meeting, as well as by participating actively with researchers of different backgrounds of the center who share their experiences.

In 2021, the following researchers from CFM joined this activity, attended by more than 300 students and 50 professionals:

- Gabriel Molina (Oral + Poster)
- Alejandro Berdonces (Oral + Poster)
- Joscha Kruse (Poster)



DONOSTIA WEEK INN 2021

donostiainn.eus/es/donostia-weekinn

18-22/11/2021

CFM regularly collaborates in the Innovation Week “Donostia WeekINN” that Fomento of San Sebastian organizes every end of October. In 2021, this collaboration was renovated again through activities for both the general public and education organized in collaboration with other institutions:

Women scientists of yesterday and today

Aquarium Donostia

Featuring Emakumeak Zientzian 2021 edition’s speakers and honored scientists.

Discovering new materials

Kursaal

Nanoscience Workshop for schools organized jointly with DIPIC and CIC nanoGUNE. 58 students participated in the 2 sessions.

OUTREACH TALKS

In addition to the events organized by CFM, several researchers of CFM participated in events organized by different institutions, giving 9 talks and reaching an overall audience of more than 1000 attendees, including the online attendance.

Outreach to get out there

Idoia Mugica Mendiola

Prisma Conference

20/05/2021

Ciencia, progreso, futuro

Ricardo Díez Muiño

Ayuntamiento Ermua

26/06/2021

La ciencia al rescate

Ricardo Díez Muiño

Summer Courses of UPV/EHU

14/07/2021

La física cuántica en la vida cotidiana

Ricardo Díez Muiño

Laboratorium Bergara

09/11/2021

Ciencia y progreso

Ricardo Díez Muiño

Aulas Experiencia UPV/EHU

18/11/2021

Las reglas del Universo

Aitor Bergara Jauregi

Helduen Hitza

21/11/2021

Pospandemia y acentos sociopolíticos: Tecnociencia y humanismo, ¿un matrimonio bien avenido?

Pedro Miguel Echenique Landibar

DIPC

15/11/2021

Unibertsoaren erregelak

Aitor Bergara Jauregi

Helduen Hitza

21/12/2021

CINEMA AND SCIENCE

Cycle organized by DIPC and Filmoteka Vasca. Presentation and discussion on the following movies:

The man who knew infinity

Pedro Miguel Etxenike Landibar

08/01/2021 Tabakalera Donostia / San Sebastián

09/01/2021 Bilbao Fine Arts Museum

Johnny got his gun

Javier Aizpurua Iriazabal

19/02/2021 Tabakalera Donostia / San Sebastián

20/02/2021 Bilbao Fine Arts Museum

The imitation game

Ignacio Arganda-Carreras and Idoia Mugica Mendiola

16/03/2021 Bilbao Fine Arts Museum



ACTIVITY IN MASS MEDIA

Press articles

38

Radio

26

Online press

99

TV

5

Many researchers were invited to participate in debates, interviews or articles in the general press.

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. To this end, Idoia Mugica Mendiola, outreach manager at CFM, and Amaia Arregi Buldain, communication technician at DIPC, collaborated with "Goiz Kronika" radio show running the section "**Zientzia Gosaria**" (Science breakfast) that is now available as a podcast.



@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 our [CFM website](#).



As of March 2022, CFM had more than 1300 followers in Twitter, 360 in Instagram, and 515 in LinkedIn. CFM's YouTube channel already contains more than 35 videos featuring different events. Besides, the CFM website is very regularly updated with news, workshops, seminars, and much more.

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 CFM 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. 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.

All the information on the GEP and its implementation is updated in CFM's webpage. Any worker can also reach the gender equality committee at any time, and a specific email account regarding equality issues is available to ensure fast and direct communication with the community: genderequality.cfm@ehu.eus.

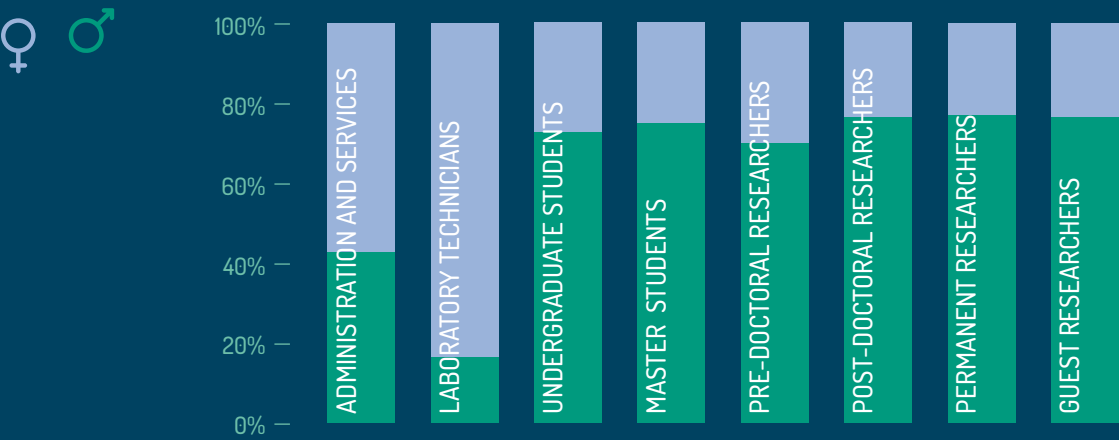
DIAGNOSIS 2021

CFM is committed to run an analysis of the internal situation yearly, publishing the compilation of its own indicators on gender balance. Data of 2021 is presented in the following table and figures:

	♀	♂	
ADMINISTRATION AND SERVICES	8	6	14
LABORATORY TECHNICIANS	5	1	6
UNDERGRADUATE STUDENTS	3	8	11
MASTER STUDENTS	2	6	8
PRE-DOCTORAL RESEARCHERS	21	49	70
POST-DOCTORAL RESEARCHERS	12	39	51
PERMANENT RESEARCHERS	11	37	48
GUEST RESEARCHERS	7	23	30
	69	169	238

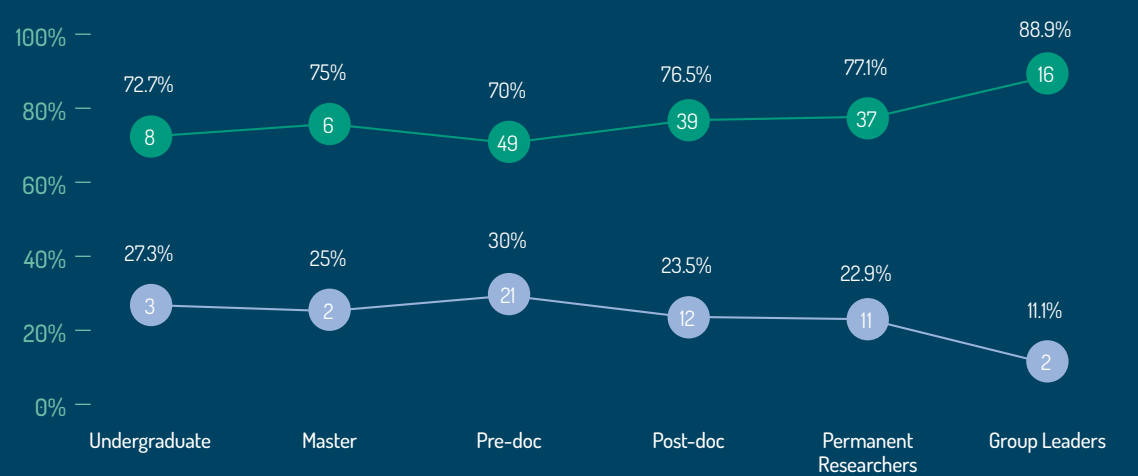
CFM is a highly masculinized workforce (71% men and 29% women at the moment), presenting vertical segregation, with women lacking at top management positions.

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



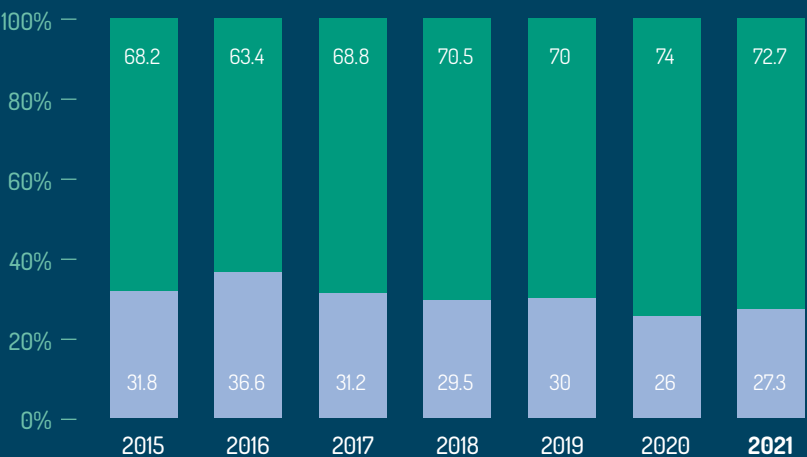
According to this data, the disproportion in the distribution of women/men in the center starts already at the earliest stage of the scientific career. Currently, 30% of the pre-doctoral researchers at CFM are women. The gender imbalance is accentuated as the responsibility for the job and level in the research career is greater, corroborating the general trend observed in the Basque Autonomous Community, Spain and Europe.

Distribution of CFM Scientific community in percentage by gender and position



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).

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



2021: First year of the implementation of the Gender Equality Plan

According to the Gender Equality Plan, there were **17 actions** foreseen for this academic year, and **88% have been in place**: 41 % of the actions were completed and 47 % of them were on track.

The aim of the plan remains to be, 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” 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, during the first year of implementation we have focused on the most urgent actions such as the design of the **Harassment Protocol**, which was launched in March 2022.



Read here the full implementation report by scanning this code or visit the Gender Equality section of the CFM website for related content.

Highlighted actions at a glance

HARASSMENT PROTOCOL

- Training on sexual harassment with an expert from Sortuz consultancy (Norma Vázquez) for all GEC members.
- Definition of CFM’s harassment policy, and development of a specific protocol.
- Designation of personal counselors: Gabriel Molina Terriza and/or Idoia Mugica Mendiola.



Read here the full Harassment Protocol by scanning this code or visit the Gender Equality section of the CFM website for related content.

INCLUSIVE USE OF LENGUAJE

- Training about the inclusive use of language at CFM.
- Development of a Decalogue of good practices.



Read here the full implementation report by scanning this code or visit the Gender Equality section of the CFM website for related content.

TRAININGS

- **TRANSFERABLE SKILLS PROGRAM. Stress Management workshop**, focused on researchers at the early stages of their careers, and Transformative Leadership, focused on senior scientists. (see the Transferable Skills program in the workshop section of this report for more information).
- **GIZONDUZ**. Face to face workshop on masculinities and the prevention of sexual and sexist harassment at work (with at least 70% of male audience, and focused on group leaders) organized by GEC and given by the Basque Government's delegation of equality.

AWARENESS

A seminar devoted to CFM community on GEP's state of the art was organized (21/05/2021), where the harassment protocol was also introduced, with the participation of more than 65 people from CFM staff.

Additionally, a new e-mail address (genderequality.cfm@ehu.eus) was created and keeps being used regularly to spread information to the entire CFM community about activities of interest related to gender equality organized by analogue institutions."

CONSOLIDATED AND REGULAR ACTIONS

- 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.

The implementation of the GEP is 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 2021 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 2022.

The current GEC is composed by:

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

MISCELLA- NEOUS



PROTEIN BASED LIGHTING TEAM WINS ROYAL SOCIETY OF CHEMISTRY'S PRESTIGIOUS NEW HORIZON PRIZE

An international collaboration of scientists, including CFM researcher Pedro Braña Coto, was awarded the Royal Society of Chemistry's new Materials Chemistry Division Horizon Prize: Stephanie L Kwolek Award. The work is a collaboration between researchers from Technische Universität München, Universität Erlangen-Nürnberg, CIC bio-maGUNE and CFM.

ARTIBLED POWERED BIOLED

The team received the prize for stabilization of fluorescent proteins in polymer coatings and their use in bio-based lighting technology. The efforts of the team on the field were already recognized and funded by the European Commission with a Fet-OPEN project, supported with more than 2.5 million euros for its development, under the title Engineered ARTificial proteins for Biological Light-Emitting Diodes (ARTIBLED).

The Horizon Prizes celebrate the most exciting contemporary chemical science at the cutting edge of research and innovation to better reflect modern science and its impacts in making the world a better place. These prizes are for teams or collaborations who are opening up new directions and possibilities in their field through ground-breaking scientific developments.



ARTIBLED powered BioLED

CFM RESEARCHER F. SEBASTIAN BERGERET SBARBARO WINS THE BESSEL AWARD OF THE HUMBOLDT FOUNDATION

The Alexander von Humboldt Foundation, established by the Federal Republic of Germany to strengthen research capabilities through international exchange, grants annually the **Friedrich Wilhelm Bessel Research Award** to **internationally renowned academics** from abroad in recognition for their outstanding accomplishments in their area of expertise and their exceptional promise for the future. As part of the prize, award winners are invited to conduct a research project of their own choosing in Germany, in close collaboration with a specialist colleague.

The winners of the Friedrich Wilhelm Bessel Award 2021 include Raúl Angulo, Ikerbasque Research Associate at Donostia International Physics Center (DIPC), and F. Sebastián Bergeret Sbarbaro, researcher at CFM.

Dr. Bergeret is known internationally for his outstanding research in quantum transport, superconductivity and related topics in condensed matter physics. He has made ground-breaking predictions on the interplay between superconductivity and magnetism in hybrid systems, which opened up new lines of research, and pioneering works on non-equilibrium superconductivity and thermoelectricity. During his stay in Germany, he will be hosted by Prof. Björn Trauzettel, at Würzburg University, to explore transport properties of two-dimensional superconducting structures with strong spin-orbit coupling.



OPEN THE DOOR TO OUR DOCTORATE CONTEST

Special **international character award** to **DOKe News team** integrated by predoctoral researchers Joscha Kruse (CFM/DIPC), Sara Luisa Marina Barbier (POLYMAT), and Stefan Merkens (CIC nanoGUNE).

In the contest "**Open the door to our doctorate**", the students of the Doctoral School (DOKe), organized in teams, presented a video aimed at promoting doctoral training at the UPV/EHU.

The team members came from 9 different countries and more than 1200 people participated in the online voting.



Watch
the video
scanning this
code

Joscha Kruse (left) and Stefan Merkens (right) at the award ceremony. Sara Luisa Marina Barbier could not attend the event.



IKUR 2030 STRATEGY

In May 2021 the Basque Government presented the IKUR 2030 strategy, addressed to institutions performing excellent science. IKUR 2030 aims at reaching international positioning of the Basque Country in strategic niches through the reinforcement of scientific capabilities. The four niches identified are **Quantum Technologies, Neutronics, High Performance Computing** and **Artificial Intelligence** (HPC+AI), and Neurobioscience.



The goal of IKUR is to maximize societal and industrial impact of the daily activity of BERCs in the field of fundamental research. Effort and resources will be focused on the four flagship fields on a sustained basis (**100 million euros will be invested in those fields during the 10 following years**). The expected impact of IKUR 2030 in terms of researchers' recruitment, publications, patents, creation of companies and associated jobs is huge, and CFM is highly committed, and exceptionally qualified, to contribute to it.

As a proof of the alignment of CFM's activity with the Basque long-term strategy for science, **CFM has been identified as a key actor in three of said IKUR fields**, and as an important collaborator in the fourth one. First of all, **CFM coordinates the IKUR field of NEUTRIONICS**, where it leads the definition and activation of a specific strategy in the Basque Country, ensuring country-wide perspective (well beyond MPC-CFM and BERCs): identifying relevant agents and roles; boosting collaboration with industry; definition of priority research lines, defining recruitment and infrastructure needs; and finally, proposing the NEUTRIONICS IKUR strategy to be adopted by the Basque Government. Secondly, under the coordination of DIPC, CFM closely collaborates in the design of the IKUR strategy for QUANTUM TECHNOLOGIES and HPC+AI fields. On top of that, even if less intensely, CFM researchers also collaborate in the definition of the strategy for the NEUROBIOSCIENCE IKUR field (coordinated by BIOFISIKA-FBB).

In the framework of the IKUR strategy, the Basque Government has granted **1 770 000 euros to MPC-CFM** to hire and train researchers, perform research projects, boost collaborations and acquire key equipment in the strategic fields mentioned in 2021, 2022 (mainly) and 2023.



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.

In the framework of this initiative, the program "Science by Women" promoted by the foundation Women for Africa, brought two African researchers to carry out six-month research stays at CFM in 2021, corresponding to the grants of 2019 and 2020 that could not be executed due to the sanitary emergency. The Provincial Council of Gipuzkoa financed each of these long stays with 25 000€.

The selected researchers were: Mary Bosede Ogundiran from Ibadan University in Nigeria (Science faculty-Chemistry department), who joined the group of Jorge Sánchez Dolado (Ceramic and Cement-Based Materials); and Abeer Mohamed Adel Mohamed Amdelbaky Elbasuony from Egypt (National Research Center, Pulp and Paper Department), who worked with Silvina Cervený Murcia at the Polymers and Soft Matter group.



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