

CFMD
CFMD
CFMD
CFMD

Materialen Fisika Zentroa
Centro de Física de Materiales
Materials Physics Center

ACTIVITY REPORT



2023

 **CSIC**
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS


Universidad
del País Vasco


Euskal Herriko
Unibertsitatea

MPC-BERC
Materials Physics Center
Basque Materials Research Center

ACTIVITY REPORT

2023

CFM

CENTRO DE FÍSICA DE MATERIALES
MATERIALEN FISIKA ZENTROA
MATERIALS PHYSICS CENTER



CONTENTS

FOREWORD	GOVERNANCE	PROFILE
06	08	10
PEOPLE	RESEARCH LINES & GROUPS	HIGHLIGHTS
12	23	39
FACILITIES & EXTERNAL SERVICES	RESEARCH OUTPUT	EDUCATION
76	84	110
WORKSHOPS, CONFERENCES, SEMINARS & COURSES	COMPETITIVE FUNDING FOR RESEARCH PROJECTS	TRANSFER OF KNOWLEDGE
117	124	142
SCIENCE AND SOCIETY	GENDER EQUALITY & DIVERSITY	MILESTONES
144	157	163

FOREWORD



Iñaki Juaristi Oleden, Vicedirector

Year 2023 was the last one for us as CFM's Director and Vicedirector. It has been a pleasure to lead CFM during these last four years, since September 2019. However, the moment has come to step down and hand over the reins to less tired hands. In our opinion, it is convenient to change leaderships with certain periodicity, so people with new, different visions can contribute to the common project. We are satisfied with the work we have performed during the last four years. During this period CFM has substantially grown: new research groups and lines have been established, and new laboratories and research infrastructures have been installed in the center. Of course, the main driven force behind these changes has been the hard work and the ambition of all the staff working at CFM. We are happy and proud to have contributed to facilitate that this evolution could take place. We also know that we are leaving CFM on the best possible hands, those of Celia Rogero as Director and Silvina Cerveny and Ion Errea as Vicedirectors. We are sure that they will do a great job leading CFM.

From the point of view of the scientific production, as you can check in this report, 2023 was again an excellent year. We 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, with 101 projects underway. The impact of CFM's scientific work keeps increasing as reflected in the number of citations of our publications: 15.220 only during 2023 and a total of 155.895 citations since the creation of the center in 1999. CFM has achieved this year an H-index of 161. We also continue with our education activity: 17 doctoral and 6 master theses were defended this year with CFM supervisors, and several undergraduate research works were supervised. We also keep increasing our technology transfer activity, favoring the creation of collaborations with private companies interested in our research and characterization capabilities. Finally, we continue our commitment to scientific outreach, this year with a record attendance to our science popularization activities.



Daniel Sánchez Portal, Director

Once more, the support obtained from the Basque Government through CFM's participation in the IKUR Strategy was crucial during 2023. This support allowed the acquisition and installation of new equipment. In particular, IKUR support was crucial to start up our new laboratory for "Materials for Quantum Technologies". This new laboratory features a dilution refrigerator capable of reaching millikelvin temperatures that became fully operational during 2023. We expect that this new facility, in addition to CFM's "Quantum Nanophotonics Laboratory", established in recent years, will allow keeping CFM at the forefront of research in the rapidly evolving field of quantum technologies in the Basque Country. IKUR Strategy also supports some of CFM's research activities in the fields of Neutron-Neutrino Science and Technologies, HPC and IA, and Nanotechnology applied to NeuroBioSciences.

During 2023 several members of CFM's scientific board obtained very prestigious awards: Angel Rubio Secade got the 2023 National Research Award; Javier Aizpurua Iriazabal, leader of CFM's Nanophotonics Theory

group, got the 2022 Euskadi Research Award; Sara Barja, received the 2023 prize awarded by Ikerbasque Foundation to the most promising female researchers (Starting level) in the Basque Country. Additionally, Josetxo Pomposo was awarded by the journal Polymer the Andrew Keller Award 2022 for his work "Starts, combs, and bottlebrushes of elastic single-chain nanoparticles".

The excellent results presented in this annual report are the result of the hard work of all the personnel at CFM. Thank you all for your commitment. Finally, it is important to remember that CFM's position as a key player in material science research is only possible thanks to the decisive and continuous support of the key institutions behind CFM-MPC: CSIC, UPV/EHU, Gipuzkoa Province Government and Basque Government. With these allies we are fully confident that we will maintain our trajectory of excellence and increase our international visibility.

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.

DIRECTION BOARD

Director: Daniel Sánchez Portal (2023) – Celia Rogero Blanco (2024)

Vice director: Iñaki Juaristi Oriden (2023) – Ion Errea Lope and Silvina Cervený Murcia (2024)

Secretary: Amaia González Azpeitia

SCIENTIFIC BOARD

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.



Centro de Física de Materiales
Materialien Fisika Zentroa



Universidad
del País Vasco

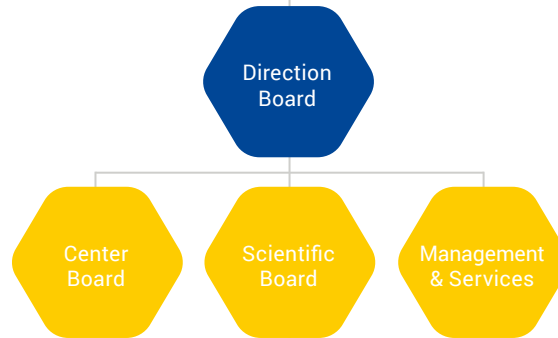
Euskal Herriko
Unibertsitatea

CSIC

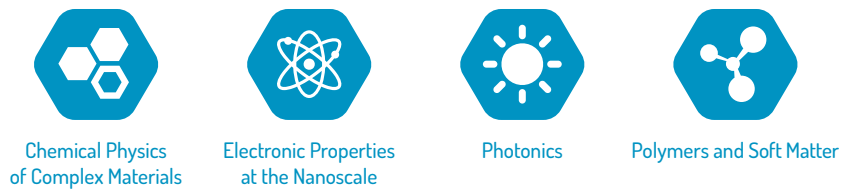
CFM



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



PROFILE



RESEARCH COMMUNITY

266

Researchers in Action

19

Research Groups



TRAINING

17

PhD Theses
defended

6

Master Theses
Defended

5

Undergraduate
Projects



RESEARCH OUTPUT

ISI Publications

211

Q1 Publications

89%

D1 Publications

40%

Open Access

84%

Citations

15 220

H Index

161

International Collaborations

76%



50%

of the Research Community is international

Researchers from

40

countries



ACTIVITIES AND EVENTS

Conferences, Workshops,
Courses, and Seminars

26

Science and Society

+70 Activities

+40 Volunteers

+12 500 Attendees



PROJECTS AND FUNDING

Ongoing Projects

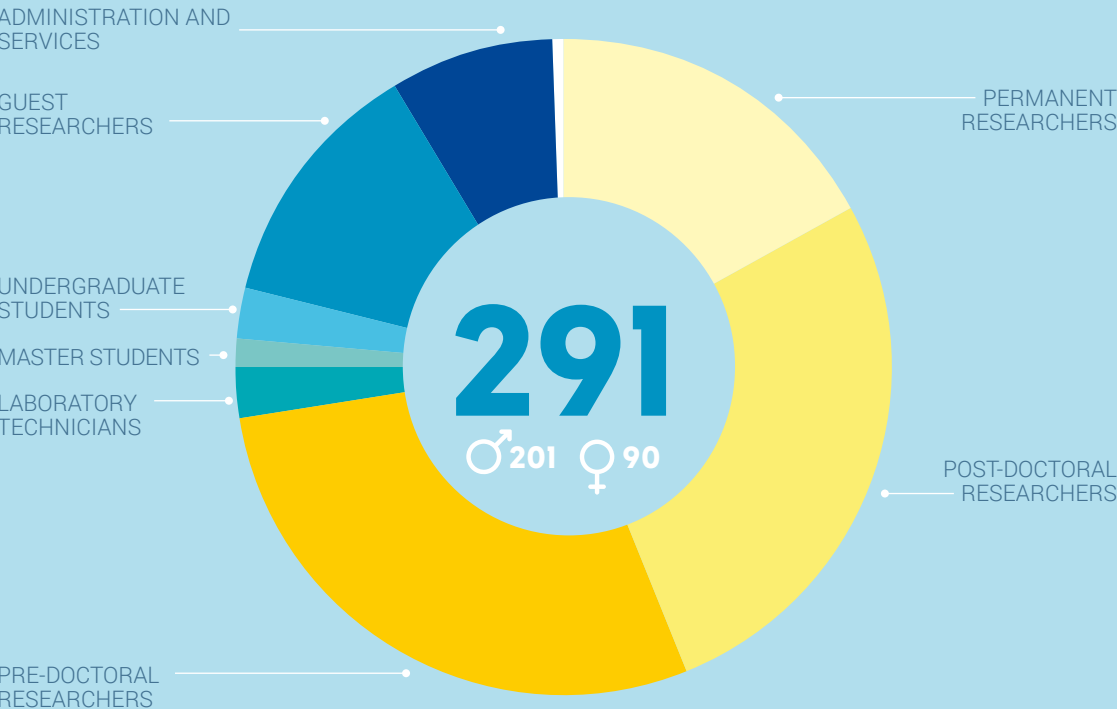
101

Funding

8 879 926.32 €

PEOPLE

ALL THE CFM COMMUNITY



Permanent Researchers	50
Post-doctoral Researchers	78
Pre-doctoral Researchers	83
Laboratory Technicians	8
Master students ¹	4
Undergraduate students	7
Guest Researchers	36
Administration and Services	24
Other guests	1
Total	291



CFM STAFF
245



RESEARCHERS IN ACTION
266²

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

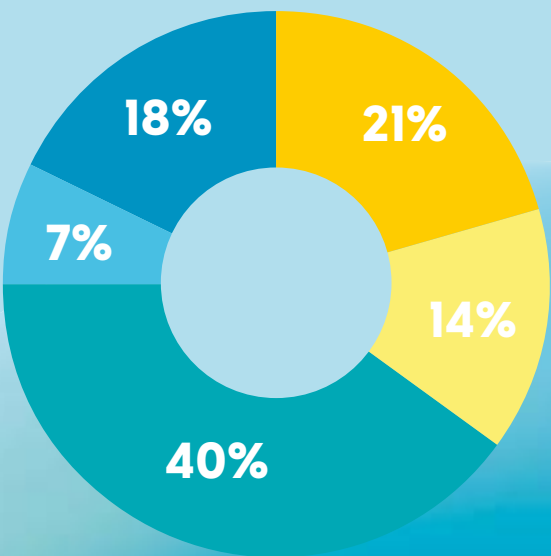
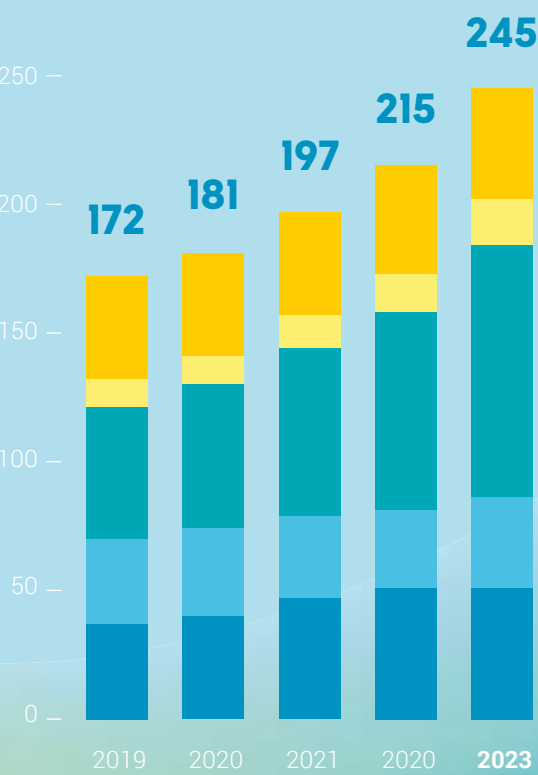
² Including Guest researchers, undergraduate and master students

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

	2017	2018	2019	2020	2021	2022	2023
CSIC	24	33	37	40	47	51	51
UPV/EHU	24	25	33	34	32	30	35
MPC-BERC	39	51	51	56	65	77	98
IKERBASQUE	7	9	11	11	13	15	18
COLLABORATORS	33	43	40	40	40	42	43
Total	127	161	172	181	197	215	245

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 2023



DIRECTION BOARD

Director: Daniel Sánchez Portal

General Manager: Amaia González Azpeitia

Vicedirector: Iñaki Juaristi Oliden



ADMINISTRATION & SERVICES

ADMINISTRATION

Adolfo del Arco García, Administrative, CSIC

Amaia Gonzalez Azpeitia, Administration Manager, CSIC

Ane Iturriza Semperena, Administrative, MPC

Annia Vázquez Fernández, Administrative, CSIC

Arantza Iturrioz Ezeiza, Project and Technology Transfer Manager, MPC

Arkaitz Nagore Ibero, Managing and Legal Director, MPC

Elixabet Sarasketa Zabala, Project and Technology Transfer Manager, MPC

Idoia Mugica Mendiola, Outreach Manager, MPC

Jon Ganuza Jiménez, Administrative, MPC

María Formoso Ferreiro, Administrative, MPC

María José Sánchez Álvarez, Executive Secretary, UPV - EHU

Marta López Pérez, Administrative, MPC

Oskitz Párraga Larrinaga, Project and Technology Transfer Manager, MPC

Tijn van den Berg, Project and Technology Transfer Manager, MPC

Txema Ramos Fernandez, Administrative, CSIC

COMPUTING AND IT SERVICES

Ander Ramos Montero, IT Systems Technician, MPC

Iñigo Aldazabal Mensa, Scientific Computing Service Manager

Ioritz Paulis Garmendia, IT Systems Technician, MPC

Irene Azáceta Elzaurdi, Scientific Computing Service, MPC

Mikel Arocena Errazquin, Scientific Computing Service, MPC

Oihan Aginaga Bote, IT Systems Internship, MPC

Urtzi Oliveras Egaña, IT Systems Technician, MPC

MAINTENANCE

Ekain Ugalde Goldarazena, MPC

Juan Manuel Burgos Jiménez, MPC

TECHNICAL STAFF

Amaia Iturrospe Ibarra, MPC

Laura Isabel Fernández Gómez-Recuero, CSIC

Luis Botana Salgueiros, CSIC

María Isabel Asenjo Sanz, MPC

Rubén González Moreno, CSIC

Silvia Arrese-Igor Irigoyen, CSIC

RESEARCHERS



Chemical Physics of Complex Materials

01 Gas/Solid Interfaces

PERMANENT RESEARCHERS

Iñaki Juaristi Oriden, *University Professor, UPV/EHU*
Maite Alducin Ochoa, *Tenured Scientist, CSIC*
Ricardo Díez Muiño, *Scientific Researcher, CSIC*

POST-DOCTORAL RESEARCHERS

Alberto Pablo Sánchez Muzas
Natalia Koval
Raúl Bombín Escudero

PRE-DOCTORAL RESEARCHERS

Alfredo Serrano Jiménez
Auguste Tetenoire
Ivan Zugec

MASTER STUDENT

Iñaki Fernández Tena

GUEST RESEARCHER

Heriberto Fabio Busnengo, *Scientific Senior*

02 Quantum Phenomena on Surfaces

PERMANENT RESEARCHERS

Nicolás Lorente Palacios, *Scientific Researcher, CSIC*
Roberto Robles Rodríguez, *Tenured Scientist, CSIC*

IKERBASQUE ASSOCIATE

Deung-Jang Choi, *MPC*

PRE-DOCTORAL RESEARCHERS

Cristina Mier González
Divya Jyoti
Mireia Tena Zuazolacigorraga

GUEST RESEARCHERS

Angel Rodríguez Alcaraz, *Pre-doctoral Researcher*
Paula Abufager, *Scientific Senior*
Eric Switzer, *Post-doc*
Román Pico, *PhD Student*

03 Nanophysics Lab

PERMANENT RESEARCHERS

Celia Rogero Blanco, *Tenured Scientist, CSIC*

Enrique Ortega Conejero, *University Professor, UPV/EHU*

Frederik Michael Schiller, *Tenured Scientist, CSIC*

Martina Corso, *Tenured Scientist, CSIC*

IKERBASQUE ASSOCIATE

Sara Barja Martínez

IKERBASQUE FELLOW

Marco Gobbi

RESEARCH COLLABORATOR

Maider Ormaza Saezmiera, *Associate Professor, UPV/EHU*

POST-DOCTORAL RESEARCHERS

Adriana Candia

Afaf El-Sayed

Andrew Patton Weber

Jesús Rubén López-Roso Redondo

John Fredy Vélez Santa

Jose Eduardo Barcelon

Maxim Ilin

Rishav Harsh

Sabine Auras

Sara Catalano

Stefano Trivini

Yuri Hasegawa

PRE-DOCTORAL RESEARCHERS

Alaa Mohammed Idris Bakhit

Alfonso Yubero Navarro

Amitayush Jha Thakur

Andrea Aguirre Baños

Carmen González Orellana

David Caldevilla Asenjo

Pablo Herrero Gómez

Paula Angulo Portugal

Rodrigo Castrillo Boderó

Samuel Kerschbaumer

Sandra Sajan

Sebastian Negrete Aragón

Sruthibhai Palakkattu Kunnu Venugopalan

GUEST RESEARCHERS

Adelina López Romers, *Undergraduate Student*

Guy Le Lay, *Scientific Senior*

Ignacio Piquero Zulaica, *Post-doctoral Researcher*

Jorge Lobo Checa, *Scientific Senior*

Marcelo Eduardo Chavez Blanco, *Pre-doctoral Researcher*

Mattia Bassotti, *Pre-doctoral Researcher*

Mikel Abadia Gutierrez, *Post-doctoral Researcher*

Sebastien Elie Hadjadj, *Pre-doctoral Researcher*

Zeinab Khosravizadeh, *Pre-doctoral Researcher*

Roser Fernández Climent, *Pre-doctoral Researcher*

Sebastien Elie Hadjadj, *Pre-doctoral Researcher*

Sergio Salaverria Bugallo, *Technician*

04 Modelisation and Simulation

PERMANENT RESEARCHERS

Andrés Arnau Pino, *University Professor, UPV/EHU*

Daniel Sánchez Portal, *Research Professor, CSIC*

RESEARCH COLLABORATOR

María Blanco Rey, *Associate Professor, UPV/EHU*

POST-DOCTORAL RESEARCHERS

Mikhail Otrokov

Samrana Kazim

PRE-DOCTORAL RESEARCHERS

Malen Etxeberria Etxaniz

Sophie Espert

GUEST RESEARCHER

Fernando Delgado Acosta, *Scientific Senior*

OTHER GUESTS

John Salusbury, *Student*

05 Spectroscopy at Atomic Scale

PERMANENT RESEARCHER

Lucia Vitali, Ikerbasque Professor, UPV/EHU

GUEST RESEARCHER

Xabier Guerrero Ricarte, Undergraduate Student

POST-DOCTORAL RESEARCHERS

Eloise Angove

Himani Malik

06 Theoretical and Computational Chemistry

PERMANENT RESEARCHER

Pedro Braña Coto, Scientific Researcher, CSIC

PRE-DOCTORAL RESEARCHER

Kalith Mohammed Ismail Syed Sulaiman

POST-DOCTORAL RESEARCHER

Irene Vettori

GUEST RESEARCHER

Luis Antonio Cabral, Post-Doctoral Researcher



Electronic Properties at the Nanoscale

07 Electronic Excitations in Surfaces and Nanostructures

PERMANENT RESEARCHERS

Andrés Ayuela Fernández, Scientific Researcher, CSIC

Eugene Tchoukov, Emeritus Professor, UPV/EHU

Pedro Miguel Echenique Landiribar, Emeritus
Professor, UPV/EHU

POST-DOCTORAL RESEARCHERS

Alberto Fraile García

Mikel Arruabarrena Larrarte

Rodrigo Humberto Aguilera del Toro

PRE-DOCTORAL RESEARCHERS

Jozef Janovec

Raúl Guerrero Avilés

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

Diego Martínez Gutiérrez
Djordje Dangic
Yuewen Fang

PRE-DOCTORAL RESEARCHERS

Antonella Meninno
Josu Diego López
Manex Alcorta Lopetegui
Martín Gutiérrez Amigo
Oscar Rodríguez Ballesteros

GUEST RESEARCHERS

Florette Corinne Fobasso Mbognou, Post-doctoral
Researcher
Jan Phillips Staller, Pre-doctoral Researcher

09 Mesoscopic Physics

PERMANENT RESEARCHER

F. Sebastián Bergeret Sbarbaro, Research Professor,
CSIC

IKERBASQUE ASSOCIATE

Vitaly Golovach, UPV/EHU

POST-DOCTORAL RESEARCHERS

Stefan Ilic
Yao Lu

PRE-DOCTORAL RESEARCHERS

Alberto Hijano Mendizabal
Jon Ortuzar Andrés

10 Nano-Bio Spectroscopy

PERMANENT RESEARCHER

Ángel Rubio Secades, University Professor, UPV/EHU

11 Souza Research Group

PERMANENT RESEARCHER

Ivo Souza, Ikerbasque Professor, UPV/EHU

IKERBASQUE FELLOW

Stepan Tsirkin

POST-DOCTORAL RESEARCHERS

Eleni Chatzikyriakou
Óscar Pozo Ocaña

GUEST RESEARCHERS

Brahim Bahloul, Scientific Senior
Cheol Hwan Park, Scientific Senior
Yangjun Lee, Pre-doctoral Researcher

12 Ceramic and Cement-Based Materials

PERMANENT RESEARCHER

Jorge Sánchez-Dolado, *Scientific Researcher, CSIC*

POST-DOCTORAL RESEARCHERS

Antoine Patt

Guido Goracci

Prodip Kumar Sarkar

Ridwan Olamide Agbaoye

PRE-DOCTORAL RESEARCHERS

Ebtisam Tarek Mohammed Saeed

Mohamad Barzegar

Mohammad Rahjoo

Rainer Bravo Pino

GUEST RESEARCHERS

Matteo Cagnoni, *Scientific Senior*

13 Theory of Electronic and Optical Excitations in Solids

PERMANENT RESEARCHER

Julen Ibáñez Azpiroz, *Ikerbasque Associate, MPC*

POST-DOCTORAL RESEARCHERS

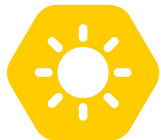
Jyoti Krishna

Peio Garcia Goiricelaya

PRE-DOCTORAL RESEARCHERS

Alvaro Ruiz Puente

Javier Sivianes Castaño



Photonics

14 Theory of Nanophotonics

PERMANENT RESEARCHERS

Javier Aizpurua Iriazabal, *Research Professor, CSIC*

Nerea Zabala Unzu, *University Professor, UPV/EHU*

Rubén Esteban Llorente, *Tenured Scientist, CSIC*

POST-DOCTORAL RESEARCHERS

Antton Babaze Aizpurua

Aurelian Loirette-Pelous

Mario Zapata Herrera

Nikolaos Iliopoulos

Sofía Isabel de Carvalho Ribeiro

PRE-DOCTORAL RESEARCHERS

Adrián Juan Delgado

Alvaro Nodar Villa

Bruno Candelas Peñalba

Carlos Maciel Escudero

Isabel Pascual Robledo

Jonathan Antonio Sepúlveda Henríquez

Xabier Arrieta Aristi

GUEST RESEARCHERS

Fernando Aguilar-Galindo Rodríguez, *Scientific Senior*

Jinna He, *Scientific Senior*

Josep Canet Ferrer, *Scientific Senior*

Mikolaj Schmidt, *Scientific Senior*

15 Nanomaterials and Spectroscopy

PERMANENT RESEARCHERS

Yuri Rakovich, Ikerbasque Professor, UPV/EHU

Marek Grzelczak, Scientific Researcher, CSIC

RESEARCHER COLLABORATOR

Ana Sánchez Iglesias

POST-DOCTORAL RESEARCHERS

Adam Olejniczak

Ane Escobar Fernández

María Sanromán Iglesias

Victor Krivenkov

PRE-DOCTORAL RESEARCHERS

Alba María Jumbo Nogales

Jehyeok Ryu

Zuzanna Lawera

GUEST RESEARCHERS

Elisa Erice Ainciburu, Master Student

Gaizka Otegi Lopez, Master Student

Heddy Wengler-Rust, Undergraduate Student

Vasily Astratov, Scientific Senior

16 Laser Spectroscopy and Photonic Materials

PERMANENT RESEARCHER

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

17 Quantum Nanophotonics Laboratory

PERMANENT RESEARCHER

Gabriel Molina Terriza, Ikerbasque Professor, MPC

POST-DOCTORAL RESEARCHERS

Alexey Brodoline

Angel Sergio Cifuentes Castro

Jason Tarunesh Francis

Jorge Olmos Trigo

Miguel Lopez Varga

Quimey Martin Pears Stefano

Rubén Pellicer Guridi

Sergio Sánchez Martín

PRE-DOCTORAL RESEARCHERS

Asier Mongelos Martínez

Iker Gómez Vilorio

Isaac Tribaldo Ramírez

Jon Lasa Alonso

María García Alonso

Martin Molezuelas Ferreras

Mikel Elorza Romera

Miriam Martínez Flórez

Shah Jee Rahman

GUEST RESEARCHER

Antonio Zelaquett Khoury, Post-doctoral Researcher





Polymers, Soft Matter & Sustainable Materials

18 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, University Professor, UPV/EHU
Gustavo A. Schwartz Pomeranec, Tenured Scientist, CSIC
Josetxo Pomposo Alonso, Ikerbasque Professor, UPV/EHU
Juan Colmenero de León, Emeritus Professor, UPV/EHU
Silvina Cervený Murcia, Tenured Scientist, CSIC

IKERBASQUE ASSOCIATE

Armando Maestro Martín

IKERBASQUE FELLOWS

Jon Maiz Sancho
Paula Malo de Molina Hernández
María Ester Verde Sesto

RAMON Y CAJAL RESEARCHER

Ivan Sasselli Ramos

POST-DOCTORAL RESEARCHERS

Alberto Álvarez Fernández
Andrey Shibaev
Beatriz Robles Hernández
Dipanwita Ghoshal
Federico Guerrero Ruiz
Jorge Humberto Melillo
Luis Alejandro Miccio Stefancik
María Dolores Ruiz Martín
Nisha Pawar Chauhan
Sebastian Bonardd Salvador
Valerio Di Lisio

PRE-DOCTORAL RESEARCHERS

Agustín Blazquez Martín
Ainara Ruiz Bardillo
Carlo Andrea Pagnacco
Carolina Iacovone
Christoph Schneck
Claudia Borredon
Davide Arena
Eric Gómez Urreizti
Francesco Coin
Javier Martínez Sabando
Jokin Pinacho Olaciregui
Leyre Oria Ledesma
Manuel Gómez Menéndez
Matteo Sanviti
Mikel Iguaran Aguirregomezcorta
Miriam Peña Figueroa
Numera Shafqat
Paschalis Agapitos
Pablo Muñumer Camacho
Sebastian Jiménez Millán
Thu Phuong Le
Vasiliki-Maria Stavropoulou

MASTER STUDENT

Jaime Blanco Caldevilla

GUEST RESEARCHERS

Ainhoa López de Uralde Baltasar, Undergraduate Student
Ayelen Cecilia Santos, Pre-doctoral Researcher
Chizoba May Obele, Post-doctoral Researcher
Diego Lecumberri Díez, Master Student
Dillip Satapathy, Scientific Senior
Lorenzo Augusto Rocchi, Pre-doctoral Researcher
Maialen Ordoñez Suquílvide, Undergraduate Student
Marta Aldecoa Ortueta, Undergraduate Student
Mathis Desseaux, Undergraduate Student
Pablo Sanchez Puga, Post-doctoral Researcher
Reidar Lund, Scientific Senior

19 Quantum Beams and Sustainable Materials

PERMANENT RESEARCHER

Felix Fernández Alonso, Ikerbasque Professor, MPC

RESEARCHER COLLABORATOR

Daniel Blanco López

POST-DOCTORAL RESEARCHERS

Kacper Druzicki

Mattia Gaboardi

Tomas Stephen Northam de la Fuente

PRE-DOCTORAL RESEARCHERS

Balthasar Braunewell

Cristina Maciá Castello

Pablo Gila Herranz

Pelayo Marín Villa

GUEST RESEARCHERS

Barbara Loska

Emma del Río Redondo

Matthias Gutmann

OTHER POSITIONS

SENIOR SCIENTISTS

Fabienne Barroso Bujans, Ikerbasque Research Professor, DIPC

Miguel Moreno Ugeda, Ikerbasque Research Associate, DIPC

POST-DOCTORAL RESEARCHER

Haojie Guo, DIPC (Miguel Moreno Ugeda's group)

Tao Wan, DIPC (Dimas García de Oteyza's group)

Wen Wan, DIPC (Miguel Moreno Ugeda's group)

PRE-DOCTORAL RESEARCHER

Alejandro Berdonces Layunta, DIPC (Dimas García de Oteyza'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, Soft Matter & Sustainable Materials-P(SM)₂**.

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 Group

Theoretical

12 Ceramic and Cement-Based Materials

Experimental

13 Theory of Electronic and Optical Excitation in Solids

Theoretical



Photonics

14 Theory of Nanophotonics

Theoretical

15 Nanomaterials and Spectroscopy

Experimental

16 Laser Physics and Photonic Materials

Experimental

17 Quantum Nanophotonics Laboratory

Experimental



Polymers, Soft Matter & Sustainable Materials

18 Polymers and Soft Matter

Theoretical and Experimental

19 Quantum Beams and Sustainable Materials

Theoretical and Experimental

Seventeen 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 “Modelisation and Simulation” group (04), and the “Theoretical and Computational Chemistry” group (06).

The other two groups in this research line develop experimental activity on the electronic properties of molecules and low dimensional structures, which are experimentally studied with the use of Scanning Tunneling Microscopy (STM) at ultrahigh vacuum and low temperature, together with a combination of Surface Physics techniques. These are the “Nanophysics Laboratory” (03) and the “Spectroscopy at Atomic Scale” (05) groups.

1

Gas/Solid Interfaces



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 calcu-

lations 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

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



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 practical 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

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 nanos-

tructures, 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

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

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



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, focusing particularly on systems of nanometer size. The general interests of this activity include: (i) spin dependent electronic excitations in oxides and metals, (ii) electronic states and excitations in topological insulators, (iii) many-body theory of electron lifetimes, (iv) basic properties, such as energy dispersion and lifetimes of novel low-energy collective excitations, and (v) studies of

nanostructures, such as two-dimensional graphene-like materials, and inorganic nanotubes and minerals containing 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

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



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

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 Group

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

In recent years, the work has involved the development of new theoretical approaches and algorithms, and their application to problems of current interest, including methods to study insulators in finite electric 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



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.

13

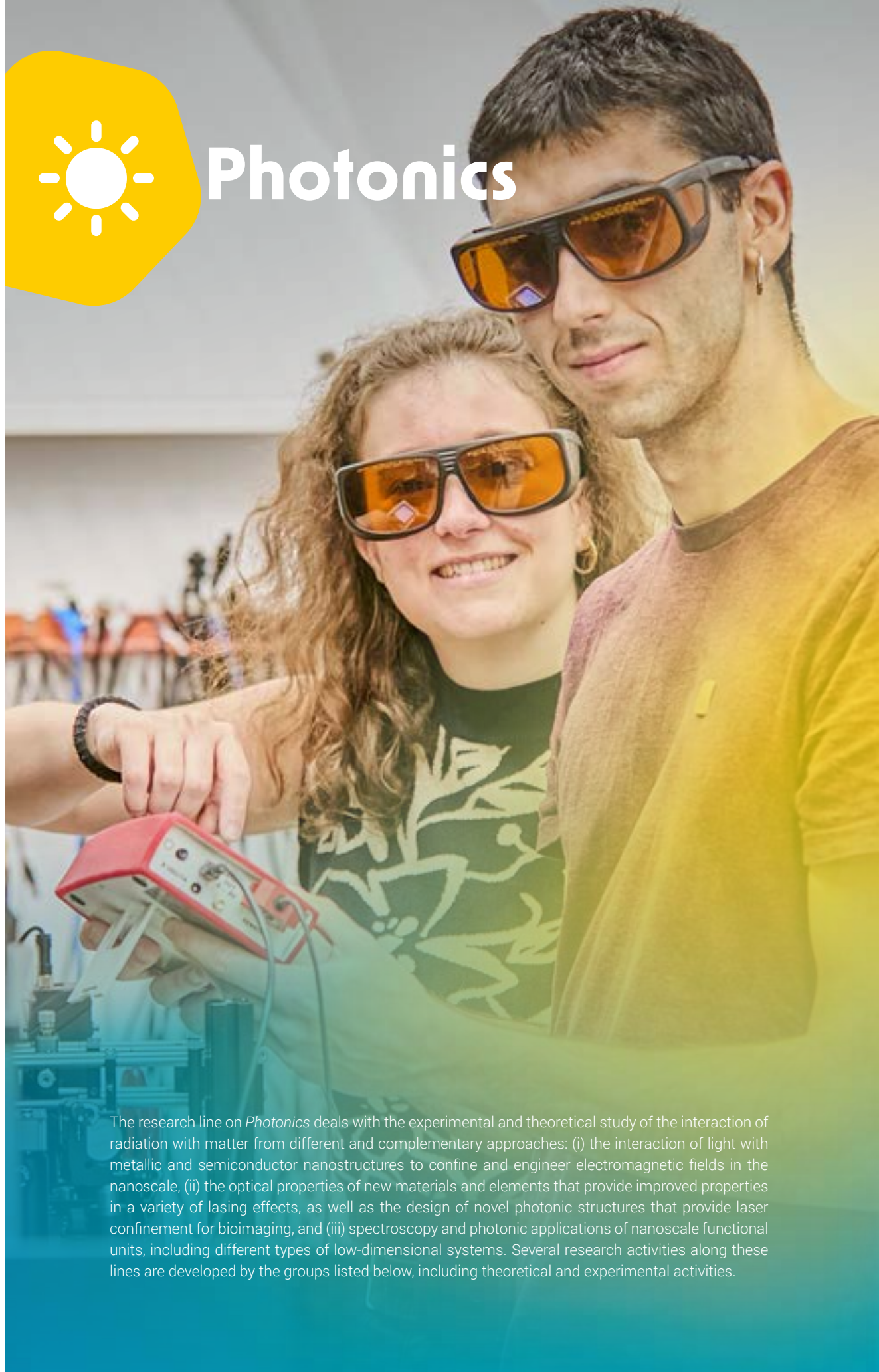
Theory of Electronic and Optical Excitation in Solids

The group’s research focuses on material properties of current interest, including (but not limited to) nonlinear optical response of semiconductors, collective electronic excitations, and magnetic behaviour of low-dimensional systems like single adatoms. For the first-principles characterization of these systems we generally make use of state-of-the-art software packages that implement the density functional theory. For the analysis of the more exotic properties we develop our own algorithms and theoretical approaches, which often make use of k-dot-p and tight-binding models.





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.

14

Theory of Nanophotonics



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

In recent years, the following specific objectives have been addressed by this group: (i) understanding and characterization of the collective excitations of 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.

15

Nanomaterials and Spectroscopy

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

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



16

Laser Physics and Photonic Materials



The activity of the **Laser Physics and Photonic Materials** group concentrates most of the research efforts on the study of light-matter interaction processes in new photonic materials with potential applications in the fields of optoelectronics (light amplifiers, lasers, light converters, laser coolers...) and biomedicine (nanostructured optical tracers, multispectral 3D images, sensors).

In recent years, the following specific objectives have been pursued on this topic: (i) the investigation on rare earth-doped vitroceraamics for integrated optics applica-

tions, (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 experimental and theoretical study of light generation in rare-earth doped micro-nano-crystalline dielectric powders for infrared random lasers, (v) the study of laser-induced refrigeration in rare earth-doped micro-nano structured materials, and (vi) the design and making up of an optical wave guide writing system by using a femtosecond laser.

17

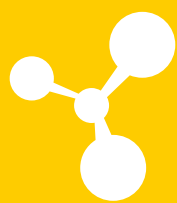
Quantum Nanophotonics Laboratory

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, Soft Matter & Sustainable Materials P(SM)₂

The research line *Polymers, Soft Matter and Sustainable Materials* combines the experimental and theoretical study of the structure and dynamics of complex molecular systems with an emphasis on polymers, soft matter and functional materials with the investigation of novel functional materials for energy applications and sustainability. In both cases Neutron Scattering and other related/complementary techniques, combined with computational methods, play a key role.

18

Polymers & Soft Matter



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.

19

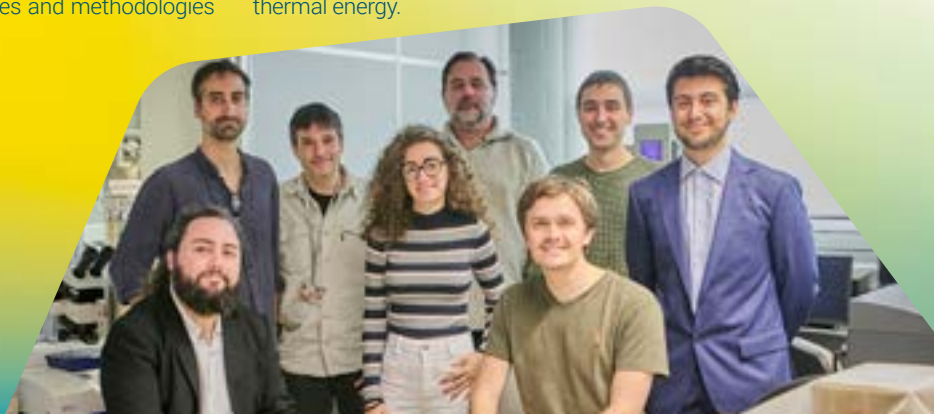
Quantum Beams & Sustainable Materials

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



HIGHLIGHTS

	PAGE
1 How adsorbed oxygen atoms inhibit hydrogen dissociation on tungsten surfaces Journal of Physical Chemistry Letters	42
2 Quantum architecture at the atomic scale: a leap forward in multi-qubit control Science 382	44
3 A ferromagnetic Eu-Pt surface compound grown below hexagonal boron nitride Nanoscale	46
4 Molecular doping in the organic semiconductor diindenoperylene: insights from many-body perturbation theory Journal of Physical Chemistry C	48
5 Thioetherification of Br-mercaptobiphenyl molecules on Au(III) Nano Letters	50
6 Dual-phosphorescent heteroleptic Silver(I) complexes in long-lasting red light emitting electrochemical cells Advance Optical Materials	51
7 Long-lived spin waves in a metallic antiferromagnet Nature Communications	52
8 Revolutionizing Electronics: Bismuth Oxide Film Stabilizes Ferroelectricity down to 1 nanometer Science 379	53
9 Ferromagnetic ordering of magnetic impurities mediated by supercurrents in the presence of spin-orbit coupling Physical Review B	55
10 A quantum-geometric theory of optical spatial dispersion in crystals SciPost Physics	57
11 Radiative Cooling Properties of Portlandite and Tobermorite: Two Cementitious Minerals of Great Relevance in Concrete Science and Technology ACS Applied Optical Materials	58

	PAGE
12 Understanding the large shift photocurrent of WS ₂ nanotubes: A comparative analysis with monolayers Physical Review B	60
13 Modifying the energy of collective molecular vibrations through optomechanical interaction Nature Communications	62
14 Thermoplasmonic self-oscillator based on gold nanoparticles Advanced Materials	64
15 Novel Sol-Gel Route to Prepare Eu ³⁺ -Doped 80SiO ₂ -20NaGdF ₄ Oxyfluoride Glass-Ceramic for Photonic Device Applications Nanomaterials 2023	65
16 Metamorphosis of a commodity plastic like PVC to efficient catalytic single-chain nanoparticles Angewante Chemie International Edition 2023	67
17 Microscopic Evidence for the Topological Transition in Model Vitrimers ACS Macro Letters	69
18 Dual crosslinking of low-methoxyl pectin by calcium and europium for the simultaneous removal of pharmaceuticals and divalent heavy metals Chemical Engineering Journal	71
19 Size-dependent vitrification in metallic glasses Nature Communications	73
20 Quantum Tunneling Rotors Unravel Gas-uptake Pathways in Metal-organic Frameworks Physical Review Materials	74

HIGHLIGHT 1

How adsorbed oxygen atoms inhibit hydrogen dissociation on tungsten surfaces

Alberto Rodríguez-Fernández, Laurent Bonnet, Pascal Larrégaray, and Ricardo Díez Muiño.

Journal of Physical Chemistry Letters 14, 1246 (2023)

Hydrogen molecules dissociate on clean W (110) surfaces. This reaction is progressively inhibited as the tungsten surface is precovered with oxygen. Ab-initio molecular dynamics calculations are used here to show that the adsorbed O atoms act as repulsive centers that modulate the dynamics of the impinging H_2 molecules by closing dissociation pathways.

Interest in the interaction between hydrogen and metal surfaces has been historically associated with heterogeneous catalysis, the basic route to any large-scale chemical industry production. Hydrogen adsorption on W is one of the simplest chemical reactions that one may envision on a surface. It has been studied for more than 100 years, since Irving Langmuir placed a filament of tungsten in a vessel containing hydrogen gas.

In spite of the extensive coverage of the problem, it is only recently that a basic atomic-level understanding of the mechanisms ruling different reactive processes of hydrogen on W surfaces has been reached. Hydrogen molecules dissociate on clean W (110) surfaces. Experiments show that this reaction is progressively inhibited as the tungsten surface is pre-covered with oxygen.

Density functional theory and ab-initio molecular dynamics are used here to rationalize, at the atomic scale, the inhibiting influence of the adsorbed O atoms on the H_2 dissociation process. In agreement with existing experimental information, the calculations show that H_2 dissociation is absent for an O coverage of half a monolayer. Therefore, the influence of O adsorbates on the dissociation dynamics on W (110) goes much beyond the blocking of possible H adsorption sites. Adsorbed O atoms create a sort of chemical shield at the surface that prevents further approach and dissociation of the H_2 molecules. Each O atom creates in its surroundings an exclusion zone for H_2 and prevents H_2 dissociation on the W atoms located in its close 3-fold vicinity.

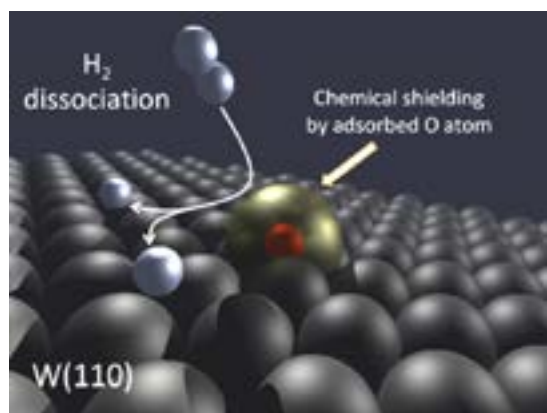


Figure 1: Illustration of the hydrogen dissociation process on W (110) when oxygen atoms are also adsorbed at the surface.

The molecular dynamics calculations show that there are actually two types of W atoms on the oxidized surface: those with an oxygen atom in their vicinity and those with no oxygen atom nearby. The former prevent H₂ dissociation while the latter provide a path to dissociation in a way similar to the clean surface. This picture may allow to extrapolate the results to other oxygen coverages, provided that phase separation exists.

All in all, ab-initio molecular dynamics calculations are a remarkable tool to understand the intricate dynamics of molecules dissociating over complex systems, such as the oxidized W (110) surface is.

"Adsorbed O atoms create a sort of chemical shield at the surface."

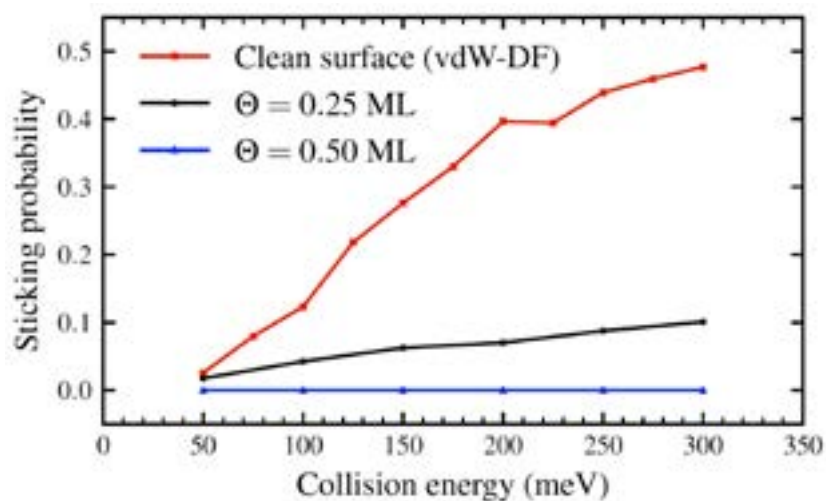


Figure 2: Dissociative sticking probabilities of H₂ on W (110) as a function of the collision energy. For all collision energies, the sticking probabilities drop as oxygen coverage of the surface increases.

HIGHLIGHT 2

Quantum architecture at the atomic scale: a leap forward in multi-qubit control

Yu Wang, Yi Chen, Hong T. Bui, Christoph Wolf, Masahiro Haze, Cristina Mier, Jinkyung Kim, Deung-Jang Choi, Christopher P. Lutz, Yujeong Bae, Soo-hyon Phark, and Andreas J. Heinrich.

Science 382, 87 (2023)

The quest for atomic-scale quantum coherence has seen a breakthrough with the realization of a multi-qubit platform. This innovation marks a pivotal advance in quantum computing, potentially reshaping the landscape of nanotechnology and quantum science.

Recent advancements in quantum technology have led to the creation of an atomic-scale platform capable of the coherent manipulation of multiple electron-spin qubits. This milestone, reported by Wang and colleagues in *Science* (2023), epitomizes the strides made in quantum science, establishing new paradigms in quantum computing and nanotechnology.

At the crux of this research is the ingenious assembly and control of electron-spin qubits at the atomic level. Achieving such precision has historically posed significant challenges due to the complexities inherent in atomic-scale operations. However, this study heralds an era of precision quantum engineering, manipulating quantum states with unprecedented control.

The platform's unique feature lies in its ability to influence qubits situated beyond the immediate vicinity of the tunnel junction. This capability is enabled by adjoining single-atom magnets that produce local magnetic field gradients, thus augmenting the electron spins. To facilitate the readout of these "remote" qubits, the team employs a sensor qubit within the

tunnel junction, executing pulsed double electron spin resonance with finesse.

This approach facilitates rapid and all-electrical operations on single, dual, and triple-qubit systems, a feat that accentuates the potential for advanced quantum functionalities. Through atom-by-atom construction on a surface, the research team has paved the way for sophisticated quantum computation, sensing, and simulation applications.

The implications of such a platform are multifaceted:

- **Quantum Computing Advancement:** This framework signifies a substantial leap toward scalable quantum computing.
- **Precise Quantum Operations:** The methodology allows for fine-tuned quantum maneuvers, enhancing computational accuracy.
- **Multi-Qubit Entanglement:** The ability to execute swift multi-qubit operations invites prospects for intricate quantum entanglement demonstrations at the Angstrom scale.
- **Versatile Quantum Systems:** The electron-spin based design permits exploration of various spin species and two-dimensional assemblies for computation and simulation.
- **Decoherence Mitigation:** The platform introduces innovative strategies to mitigate decoherence, thereby extending energy relaxation and coherence times.

"The atomic-scale qubit platform crafted by researchers at four international institutions including CFM presents a groundbreaking leap in quantum science, enabling precise and coherent quantum operations at the single-atom level."

In essence, the study sets a new standard for quantum control, potentially catalyzing advancements in both quantum science and nanotechnology. This atomic-scale qubit platform not only redefines current quantum computational paradigms but also emboldens the future of quantum applications, promising an era of heightened precision and efficiency.

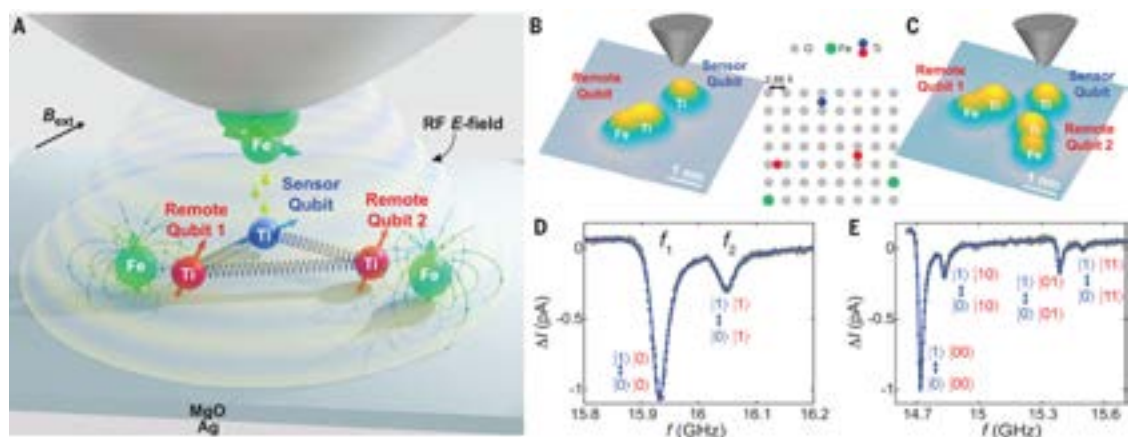


Figure: Bottom-up construction of multiple coupled electron spin qubits.

(A) Schematic: A sensor spin qubit (Ti, blue) is placed under the apex of a spin-polarized STM tip for readout. Remote qubits are constructed at precise separations to the sensor qubit by atom manipulation. Each remote qubit is composed of a spin-1/2 Ti atom (red) and a single-atom magnet (Fe) (green), where Fe's magnetic field gradient, in combination with the RF electric field between the tip and the sample, coherently drives remote qubits. (B and C) Constant-current STM images showing atom-by-atom construction of a multi-qubit structure composed of two (B) and three (C) qubits (image size: 5.0×5.0 nm). Inset: atomic registry of the structure in (C). Structure in (B) has the same configuration but without remote qubit 2. (D and E) Continuous-wave ESR spectra measured with the tip positioned on the sensor qubit in the two-qubit (D) and three-qubit (E) structure. The quantum states of the sensor qubit are labeled by the first kets. Each ESR transition of the sensor qubit distinguishes a quantum state of the remote qubits (the second kets). The measured spin-polarized tunnel-current signal ΔI is the difference between averaged signals in lock-in A and B subcycles (fig. S10), which reflects the change of the sensor spin polarization due to applied coherent control pulses [see section 4 of (19)]. Imaging conditions in (B) and (C): sample bias voltage VDC = 100 mV, time-averaged tunnel current IDC = 10 pA. ESR conditions in (D) and (E): VDC = 50 mV, IDC = 20 pA, zero-to-peak RF voltage VRF = 30 mV. The sample was kept at 0.4 K during measurements.

HIGHLIGHT 3

A ferromagnetic Eu-Pt surface compound grown below hexagonal boron nitride

Alaa Mohammed Idris Bakhit, Khadiza Ali, Anna A. Makarova, Igor Piš, Federica Bondino, Roberto Sant, Saroj P. Dash, Rodrigo Castrillo-Bodero, Yuri Hasegawa, J. Enrique Ortega, Laura Fernandez, and Frederik Schiller.

Nanoscale 15, 11517 (2023)

Europium is a very interesting element having the ability to occur in a di-, a tri-, or a mixed-valence state. Divalent Eu has a half filled 4f shell and is magnetic while tri-valent Eu is nonmagnetic. We can produce a ferromagnetic Eu-Pt surface alloy by Eu atom intercalation under a 2D hexagonal boron nitride (hBN) monolayer grown on a curved Pt crystal. The hBN coat protects partially the Eu from oxidation, allowing to retain its magnetic properties.

Ferromagnetic two-dimensional (2D) structures are of uttermost importance in spintronics applications. Such 2D magnetic systems can either be 2D van der Waals (vdW) ferromagnets, or ultrathin magnetic overlayers. Both types of systems present quantum and topological phases, but achieving new exotic properties requires design and investigation of novel materials and architectures. In thin magnetic overlayers, transition and/or rare-earth metals are commonly used. The interest in such 2D ferromagnetic systems is prompted by the re-

duced atomic-scale size and the diversity of magnetic states that arise. Nevertheless, being surface systems they may be subject to oxidation or contamination. One has to find intelligent approaches to protect such 2D ferromagnetic systems from unwanted environmental modifications. Here, we study a hBN-protected ferromagnetic Eu-Pt surface alloy. The Eu-Pt compound is formed after Eu intercalation under the hBN film previously grown on a Pt crystal surface, see Figure 1 for a schematic description of the experiment.

The substrate material is a cylindrical sector of a single Pt crystal. Across the curved side of the cylinder, the surface features different crystal facets with an increasing density of steps. We expose the substrate hold at 700°C to borazine vapor to form the hBN monolayer. Then we verify the electronic properties by X-ray and angle-resolved photoemission spectroscopy (XPS, ARPES), as well as the structure by low energy electron diffraction and scanning tunneling microscopy. The next step is depositing a small amount of Eu at an elevated temperature. This procedure allows Eu to directly intercalate via wrinkles or grain boundaries of the hBN layer, such as to form an EuPt₂ subsurface compound.

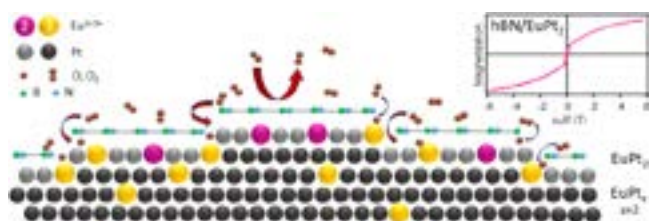


Figure 1: Schematic description of the experimental system. A curved Pt single crystal around the (111) face is used for hBN growth. Eu is intercalated below the hBN forming a ferromagnetic EuPt₂ surface compound. After air exposure, the (111) part of the EuPt₂ can be protected, at the vicinal parts the protection is strongly reduced.

Our investigations reveal that the majority of Eu stays at the hBN/Pt interface forming the mentioned EuPt₂ compound that is ferromagnetic (Curie temperature TC approx. 20 K), with Eu in a divalent state. Part of the Eu further migrates to the Pt bulk forming the non-magnetic, tri-valent Eu-Pt alloy. These results are shown in Figure 2(a) and (b).

Last, we expose this heterolayer system to ambient conditions to check if the very reactive interface Eu atoms are chemically protected by the hBN layer on top. For this, we check again XPS and ARPES at the Pt(335), Pt(111) and Pt(332) facets of the curved Pt substrate, see Figure 2(c). The spectroscopy results in part (d) of Figure 2 indicate that part of the divalent Eu atoms in the EuPt₂ interface are protected from air at the (111) and the (335) positions.

"A ferromagnetic EuPt₂ surface compound is formed by intercalation through a hexagonal boron nitride monolayer grown on a curved crystal Pt sample. At the (111) and (335) positions the magnetic surface compound is partially protected from oxidation by air exposure"

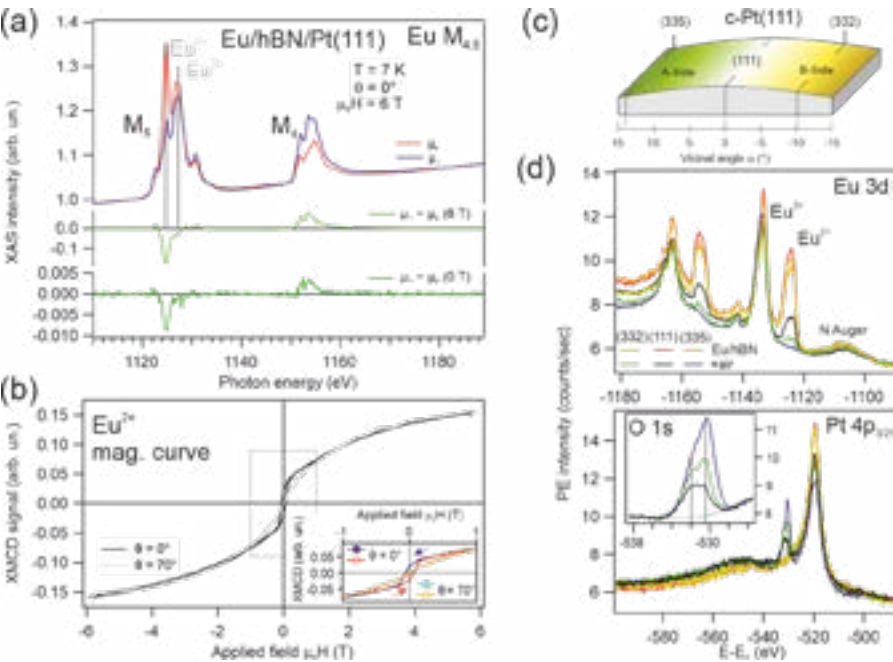


Figure 2: Magnetic and electronic properties of EuPt₂ surface compound protected by hBN. (a), (b) X-ray absorption and X-ray magnetic dichroism spectra and magnetization curves at the Eu $M_{4,5}$ absorption edge confirming the ferromagnetic state of Eu. (c) Schematic description of the curved substrate. (d) X-ray photoemission spectroscopy prior and after air exposure of the hBN/EuPt₂ system, revealing partial chemical protection at (111) and (335) surfaces.

HIGHLIGHT 4

Molecular doping in the organic semiconductor diindenoperylene: insights from many-body perturbation theory

Masoud Mansouri, Peter Koval, Sahar Sharifzadeh, and Daniel Sánchez-Portal.

Journal of Physical Chemistry C 127, 16668-16678 (2023)

In this study we use the GW/BSE (GW+ Bethe-Salpeter equation) approach to study the effect of molecular doping on organic semiconductors. Our results highlight the importance of accurately taking into account the solid-state screening and dopant-host interactions in order to satisfactorily describe the optoelectronic properties of those systems.

In this study we take advantage of the quantitative accuracy of the GW/BSE approach to describe the electronic structure and optical properties of an interesting organic semiconductor (OSC): diindenoperylene (DIP) molecular crystal. We focus on the doping of DIP crystals with acceptor molecules in order to control their carrier density and mobility. This is crucial to tune the conductivity and optical properties of this material for specific applications. Our results clearly indicate that, contrary to the customary belief, neither the information obtained from the isolated molecules nor from molecu-

lar crystals in the pure phase is sufficient to determine relevant dopant-host combinations. The interaction and hybridization with the host environment, including many-body effects, must be carefully considered in order to successfully identify appropriate molecular dopants for a given OSC. Fortunately, our paper demonstrates that the accuracy of current GW/BSE methods can be sufficient to allow identifying such dopants.

We first show that our theoretical estimates of the transport and optical gaps, as well as the optical absorption spectra, of the isolated and the crystalline DIP are in excellent agreement with available experimental data. We then perform a systematic analysis of the dopability of the DIP with two strong acceptors, namely F4TCNQ and F6TCNNQ molecules. Our analysis demonstrates that the studied doped crystals feature hybridized states at the valence-band edge associated with a host-dopant charge-transfer complex that must be taken into account in order to understand the electronic and optical properties of the system. Additionally, electrostatic and solid-state screening effects are instrumental in accurately describing the level alignment between dopant and host molecules.

In summary, we propose two new doped DIP crystals with salient features in their optical structures that could be exploited for optoelectronic applications. Furthermore, our results disprove the belief that the ionization energy and the electron affinity computed in the gas phase or even measured on films of pure host and dopant molecules can be applied to discuss the dopability of an OSC. In contrast, we demonstrate that environmental screening and interaction effects must be carefully taken into account to obtain a reliable picture of the doping of molecular crystals.

"Our results clearly indicate that, contrary to the customary belief, neither the information obtained from the isolated molecules nor from molecular crystals in the pure phase is sufficient to determine relevant dopant-host combinations"

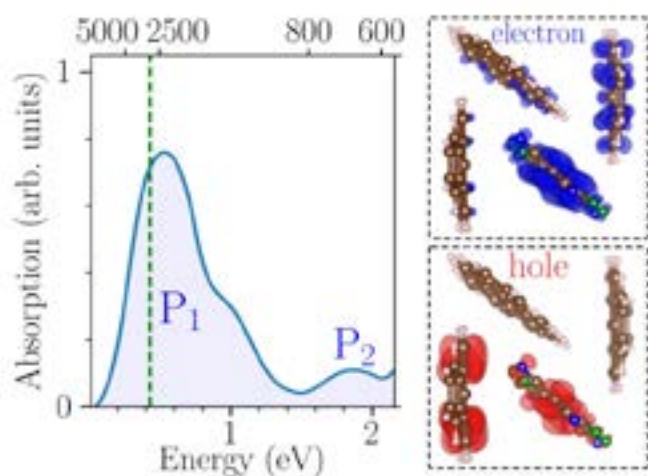


Figure: (Left) Low energy optical absorption spectrum of the DIP crystal substitutionally doped with F6TCNNQ. (Right) Scheme showing the unit cell containing three DIP molecules and one F6TCNNQ molecule, together with the spatial distribution of the hole/initial-state (red) and electron/final-state (blue) densities for the P_1 peak. Note that the hole density is mainly centered on the HOMO of one of the host DIP molecules, while the electron density shows a large contribution from the LUMO of the dopant molecule. In spite of the hybridization between neighboring molecules, this highlights the dominant host-dopant charge-transfer character of the P_1 transition.

HIGHLIGHT 5

Thioetherification of Br-mercaptobiphenyl molecules on Au(111)

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

Nano Letters 23, 1350-1354 (2023)

Scanning tunneling microscopy has emerged as a powerful tool that significantly contributes to our understanding of chemical reactions, particularly in visualizing catalytic reaction steps on surface templates. These investigations have played a crucial role in clarifying the reaction steps leading to the synthesis of nanostructures with desired shapes and electronic properties, which are essential for advancing quantum technologies.

Despite its relevance and success in unravelling reaction steps, most investigations focused on synthesizing polymeric nanostructures using molecular precursors with a single functionalized reacting group. For example, graphene nanostructures are primarily formed on metal surfaces through the thermal activation of molecular de-halogenation followed by carbon-carbon coupling between adjacent molecules. Thiols, instead, most often dehydrogenate leading to strong chemical bonds to metal surfaces. The strength of this bond is such that thermal activation rather induces the detachment of chalcogen atoms from organic structures. Investigations exploring on-surface reaction steps between molecular precursors holding simultaneously these two groups have not been undertaken yet.

In a collaborative effort between CFM, Ikerbasque, and DIPC, molecular C-S bonds were successfully formed on Au (111) surfaces using molecular precursors functionalised with both halogen and a sulfhydryl group. This introduces an important novelty to the field of surface synthesis. The reaction leads exclusively to the thioetherification of the molecules despite the two mentioned competing reactions. Extended polymeric chains, characterized by new chemical C-S bonds are observed upon thermal activation of 4'-Bromo-4-mercaptobiphenyl molecular precursors adsorbed on the Au surface.

The authors identified four reaction steps involving sulfhydryl or bromine molecular groups leading to intermolecular C-S bond formation, through scanning tunneling microscopy, spectroscopy, and first-principles calculations. The study shows that to form the thioether polymer and overcome the common competitive formation of C-C bonds, two of these reaction steps, namely the dehalogenation and dissociation of the S-Au bond, must occur simultaneously. This research provides insights into such polymeric structure synthesis, revealing changes in precursor electronic properties upon bonding and molecular precursor length.

"Exploring new pathways in the surface synthesis of polymers and covalent bonding"



Figure: Schematic representation of the thermally induced thioetherification process of 4'-Bromo-4-mercaptobiphenyl (Br-MBP) molecules on the Au (111) surface. The presence of S atoms strongly modulates the electronic properties of the phenyl chain.

HIGHLIGHT 6

Dual-phosphorescent heteroleptic Silver(I) complexes in long-lasting red light emitting electrochemical cells

Sophia Lipinski, Luca M. Cavinato, Thomas Pickl, Giulia Biffi, Alexander Pöthig, Pedro B. Coto, Julio Fernández-Cestau, and Rubén D. Costa.

Advance Optical Materials 11, 2203145 (2023)

We have designed the [Ag(xantphos)(deebq)]PF₆ complex combining a large-bite angle diphosphine ligand (xantphos) and a rigid, sterically hindered, π -extended biquinolin (deebq). With this complex, we have developed the first red light-emitting electrochemical cells featuring improved stability of two orders of magnitude compared to prior-art.

The design of red-emitting silver (I) complexes and their implementation in thin-film lighting are still challenging as i) their high ligand-field splitting energy leads to high-energy emissions with a controversial mechanism (thermally activated delayed fluorescence vs. fluorescence/phosphorescence), and ii) their low electrochemical stability leads to the formation of silver nanoclusters, limiting the device stability to a few seconds. Herein, we report a thoughtful complex design

[Ag(Xantphos)(deebq)]PF₆ combining a large-bite angle diphosphine ligand (Xantphos) and a rigid, sterically hindered, and π -extended biquinolin (deebq). In sharp contrast to prior-art, this complex possesses i) efficient red-emission (π_{em} =660 nm; photoluminescence quantum yield of 42%) assigned to a thermally equilibrated dual-phosphorescent emission based on spectroscopic/theoretical studies and ii) stable reduction behavior without forming silver nanoclusters. This results in the first red light-emitting electrochemical cells featuring i) an improved stability of two orders of magnitude compared to the prior-art (from seconds to hours) at irradiances of 20 mW/cm², and ii) a new degradation mechanism exclusively related to p-doping as confirmed by electrochemical impedance spectroscopy analysis. Indeed, a multilayered architecture to decouple hole injection/transport and exciton formation enabled a further 2-fold enhanced irradiance/stability. Overall, this work illustrates that deciphering the rules for silver(I) complex design for lighting is tricky, but worthy.

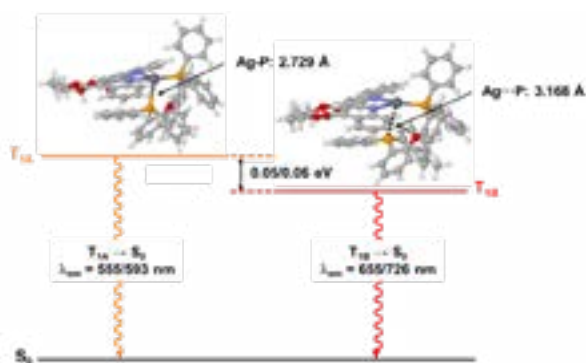


Figure: Schematic representation of the equilibrium structures of the triplet excited states of [Ag(Xantphos)(deebq)] involved in the emission process, the experimentally obtained/calculated values of the emission wavelengths and the energy gap highlighting the thermal equilibration situation responsible for the dual phosphorescence observed in this system.

HIGHLIGHT 7

Long-lived spin waves in a metallic antiferromagnet

Poelchen G, Hellwig J, Peters M, Usachov DY, Kliemt K, Laubschat C, Echenique PM, Chulkov EV, Krellner C, Parkin SSP, Vyalikh DV, Ernst A, and Kummer K.

Nature Communications 14, 5422 (2023)

A metallic antiferromagnet CeCo_2P_2 is sustaining long-lived terahertz magnons due to suppressed low-energy spin-flip excitations, as shown by first-principle calculations and resonant inelastic X-ray scattering. Our findings highlight the potential for bulk metallic systems to support undamped terahertz magnons, promising for next-generation spintronic devices.

Collective spin excitations in magnetically ordered crystals, called magnons or spin waves, can serve as carriers in novel spintronic devices with ultralow energy consumption. The generation of well-detectable spin flows requires long lifetimes of high-frequency magnons. In general, the lifetime of spin waves in a metal is substantially reduced due to a strong coupling of magnons to the Stoner continuum. This makes metals unattractive for use as components for magnonic devices. Here, we present the metallic antiferromagnet CeCo_2P_2 , which exhibits long-living magnons even in the terahertz (THz) regime. For CeCo_2P_2 , our first-principle

calculations predict a suppression of low-energy spin-flip Stoner excitations, which is verified by resonant inelastic X-ray scattering measurements. By comparison to the isostructural compound LaCo_2P_2 , we show how small structural changes can dramatically alter the electronic structure around the Fermi level leading to the classical picture of the strongly damped magnons intrinsic to metallic systems. Our results not only demonstrate that long-lived magnons in the THz regime can exist in bulk metallic systems, but they also open a path for an efficient search for metallic magnetic systems in which undamped THz magnons can be excited.

“Metallic antiferromagnets like CeCo_2P_2 can sustain long-lived terahertz magnons, offering new possibilities for efficient spintronic devices”

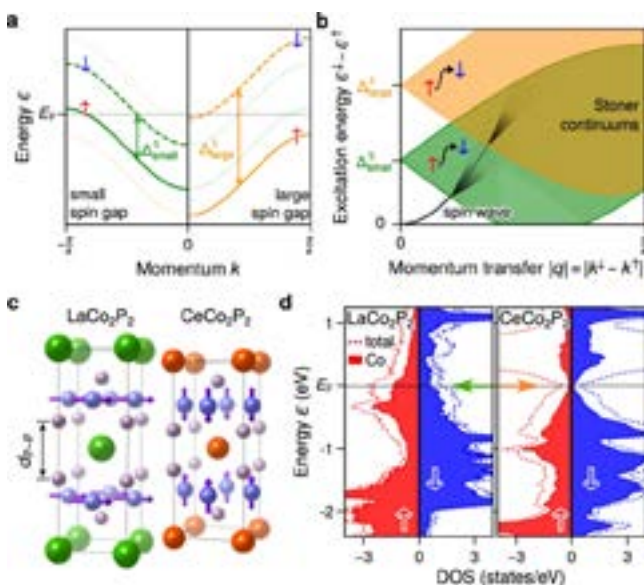


Figure: **a** Metallic band structure of a spin-split band for a small and large spin (Stoner) gap. **b** Relationship between the corresponding Stoner continuum and the onset of the spin wave scattering. Larger spin gaps promote undamped spin waves up to higher energies. **c** Crystal structure of LaCo_2P_2 and CeCo_2P_2 with the reduced distance and larger magnetic exchange between Co layers in CeCo_2P_2 . **d** Spin-resolved density of states in LaCo_2P_2 and CeCo_2P_2 .

HIGHLIGHT 8

Revolutionizing electronics: bismuth oxide film stabilizes ferroelectricity down to 1 nanometer

Qianqian Yang, Jingcong Hu, Yue-Wen Fang, Yueyang Jia, Rui Yang, Shiqing Deng, Yue Lu, Oswaldo Dieguez, Longlong Fan, Dongxing Zheng, Xixiang Zhang, Yongqi Dong, Zhenlin Luo, Zhen Wang, Huanhua Wang, Manling Sui, Xianran Xing, Jun Chen, Jianjun Tian, and Linxing Zhang.

Science 379, 1218 (2023)

This research presents a breakthrough in the field of atomic-scale ferroelectrics by demonstrating the stability of ferroelectricity in a layered film of bismuth oxide down to 1 nanometer through samarium bondage. The research findings have been published in the journal Science, where Linxing Zhang from the University of Science and Technology Beijing and Yue-Wen Fang from CFM led the experimental and theoretical work, respectively.

Ferroelectrics exhibit spontaneous electric polarizations that can be reversed by an external electric field. They have been applied into information storage, sensors and ultrasound devices. Nowadays, the ferroelectric industry is valued at approximately \$7 billion and continues to grow. The CFM researcher Dr. Yuewen Fang has collaborated Dr. Linxing Zhang at the USTB to design a new ferroelectric material that pushes the size down to the atomic scale. The work has been published today in Science.

The material, which consists of a layered structure of bismuth oxide stabilized by samarium bonding, shows a remanent polarization of up to 17 microcoulombs per square centimetre even at thicknesses as small as 1 nanometer. It has a high Curie temperature of approximately 500 K, making the room-temperature applications possible.

The crystal structure prediction was primarily led by CFM and involved a collaboration with Dr. Oswaldo

Dieguez at Tel Aviv University. The theoretically proposed crystal structure is in a good agreement with the cross-sectional high-angle annular dark-field scanning transmission electron microscopy images observed in different directions, implying the accuracy of the crystal structure prediction (see Figure 1).

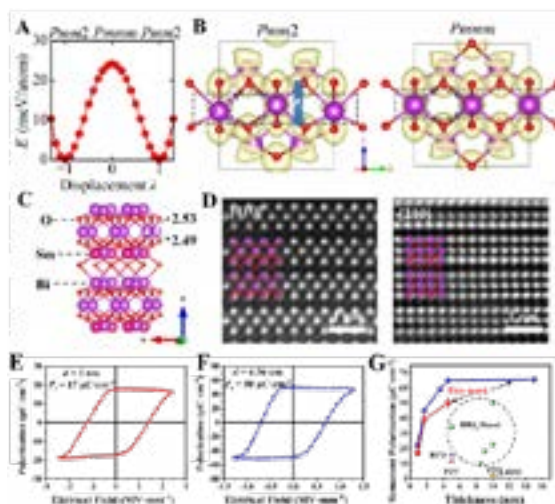


Figure 1: The proposed crystal structure and the interpretation of ferroelectricity. (A) The computed ferroelectric transition between the polar and non-polar structures. (B) The electron localization function of the two phases demonstrating the role of long-pair electrons of Bi in driving the ferroelectricity. (C) The Sm doped Bi₆O₉ structure in which the polar symmetry is preserved. (D) The comparison between the theoretical structure and the HAADF-STEM images. (E and F) The polarization hysteresis loops of the films with thicknesses of 1 nm (E) and 4.56 nm (F). (G) The comparison with other ferroelectric systems in remanent polarization.

The first-principles calculations revealed that the ferroelectricity is driven by the lone-pair electrons of Bi ions. These electrons are resided in one side of Bi ions asymmetrically, which breaks the inversion symmetry and induces the ferroelectricity. In addition, the study also finds that the doping of samarium into the sample is crucial for the thermodynamic stability of the polar structure especially when the size is reduced to 1 nanometer, according to the ab initio molecular dynamics simulations by Dr. Fang.

Overall, these ultrathin ferroelectric films are highly suitable for future nano-electronic devices, particularly in the areas of field-effect-transistors, low-power logic, and non-volatile memories. The structure design of these films has enormous potential for manufacturing atomic-scale electronic devices. In fact, the team has achieved a giant tunnelling electroresistance of 700,000 in the atomic-scale ferroelectric tunnel junctions based on the above material very recently (See Nature Communications).



Figure 2: *The future subnanometer untrathin memory devices based on atomic scale ferroelectrics.*

HIGHLIGHT 9

Ferromagnetic ordering of magnetic impurities mediated by supercurrents in the presence of spin-orbit coupling

Yao Lu, Ilya Tokatly, and F. Sebastian Bergeret.

[Physical Review B 108, L180506 \(2023\)](#)

Usually conventional superconductivity and ferromagnetic ordering are considered antagonistic effects. In contrast to this conventional understanding, our study reveals long-range ferromagnetic interactions between magnetic impurities in superconductors with spin-orbit when taking into account the influence of the electromagnetic field.

Ferromagnetic ordering is often seen as incompatible with conventional superconductivity due to the presence of an effective exchange field in ferromagnets. This exchange field has the effect of breaking up Cooper pairs, which are composed of electrons in a singlet state. The coexistence of these two orders, however, does exist in hybrid superconductor/ferromagnet (S/F) structures. In ferromagnet/superconductor/ferromagnet (F/S/F) structures, the energetically favorable arrangement is an antiparallel orientation of the magnetizations of the two F regions. This situation changes in thin superconducting films with spin-orbit coupling (SOC). The combination of the exchange field generated by a magnetic impurity (m_1 in Figure 1) and the SOC results in the spontaneous generation of anomalous currents through the spin-galvanic effect. In the case of a Rashba SOC, they flow perpendicular to the magnetization. The orientation of the third magnetic moment of a second impurity (m_2 and m_3 in Figure 1) is determined by minimization of the free energy: To reduce the kinetic energy of the superflow they will generate anomalous currents that suppress the currents induced by m_1 .

Consequently, m_2 will point in the positive x direction and m_3 to the negative x direction. In other words, the supercurrent mediated magnetic interaction is ferromagnetic between m_1 and m_2 while it is antiferromagnetic for m_1 and m_3 . Previous studies on Rashba superconductors have obtained an interaction resembling the 2D DDI form, which does not result in either a ferromagnetic or an antiferromagnetic ground state for two impurities. However, those studies have neglected the influence of the electromagnetic (EM) field.

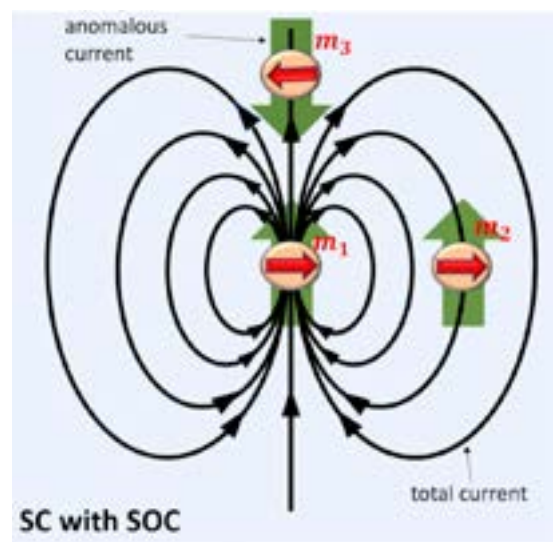


Figure 1: Schematic plot of magnetic impurities on top of a superconductor thin film with spin-orbit coupling. The red arrows represent the magnetization of the impurities. The green arrows are the exchange field-induced localized anomalous currents. The black loop represents the total current induced by the exchange field, phase gradient, and electromagnetic field.

In this work, we present a theory elucidating the impact of the electromagnetic field on the magnetic coupling between impurities. We predict a ferromagnetic coupling between two impurities in superconducting systems with SOC. In a Bravais lattice (Figure 2) of magnetic impurities, superconductivity mediates the establishment of ferromagnetic order within specific parameter ranges. These findings challenge the conventional understanding that ferromagnetism and superconductivity are mutually exclusive phenomena. Our theoretical framework provides a plausible explanation for the recently observed remanent flux and transport signature of ferromagnetism in iron-based superconductors, particularly Fe(Se,Te).

“This study reveals long-range ferromagnetic interaction between two impurities, mediated by the interplay between the superfluid response ions and the anomalous supercurrents due to magnetoelectric effects”

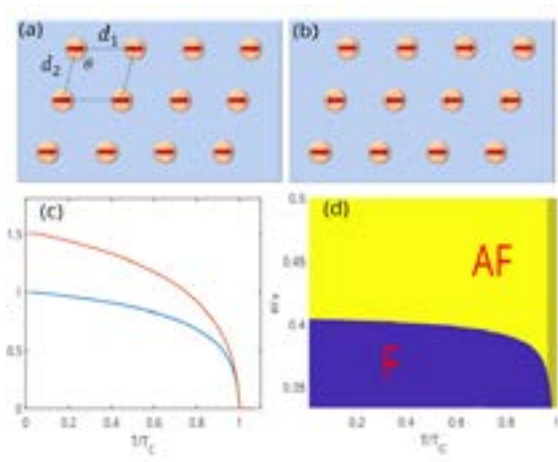


Figure 2: (a), (b) Schematic picture of the ferromagnetic and the layered antiferromagnetic states of a Bravais magnetic impurity lattice. (c) Temperature dependence of the interaction strength. The red line and blue line denote parallel and perpendicular coupling respectively. (d) Phase diagram for a 2D impurity lattice.

HIGHLIGHT 10

A quantum-geometric theory of optical spatial dispersion in crystals

Óscar Pozo Ocaña, and Ivo Souza.

[SciPost Physics 14, 118 \(2023\)](#)

The light-matter interaction is often treated by setting the wave vector $q=2\pi/\lambda$ to zero. While this is an excellent approximation for many purposes because λ is typically much larger than atomic dimensions, it fails to capture phenomena such as natural optical activity, the rotation of the plane of polarization of light as it travels through a chiral medium, depicted in the figure.

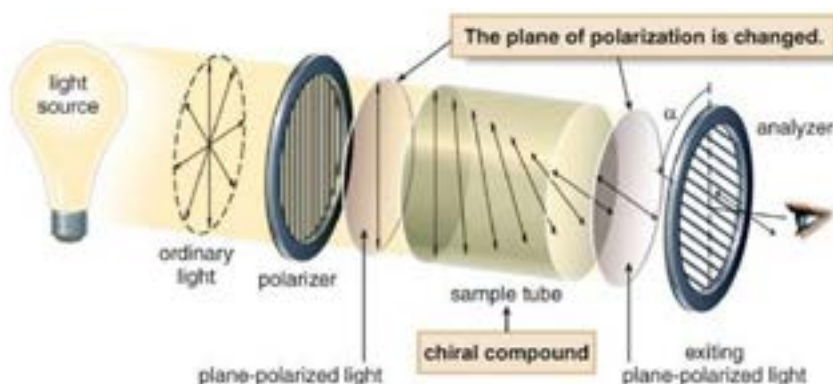
Such spatially-dispersive effects originate in the weak spatial inhomogeneity of the electromagnetic field on the atomic scale. In molecules, they are described by the multipole theory of electromagnetism, where the coupling to light is treated by including terms beyond the electric-dipole (or infinite-wavelength) approximation. That theory has two shortcomings: it is limited to bounded systems, and its building blocks – the multipole transition moments – are origin dependent.

In this work, we develop a quantum-geometric theory of optical spatial dispersion in crystals.

Working in the independent-particle approximation, we introduce intrinsic multipole transition moments

that are origin independent and transform covariantly under gauge transformations of the Bloch states. Electric-dipole transitions are given by the Berry connection, while magnetic-dipole and electric-quadrupole transitions are described by the intrinsic magnetic moment (spin plus orbital) and by the quantum metric of the Bloch states, respectively. In addition to multipole-like terms, the optical response of crystals at first order in q contains additional terms proportional to the band velocity that have no counterpart in molecular theories.

A neat outcome of this theory is a topological rotatory-strength sum rule. It has been known since the early days of quantum mechanics that the rotatory strength of chiral molecules (the difference in absorption strength of left- and right-circularly polarized light) sums to zero over all optical transitions. We have found that this sum rule remains valid for optically-active metals for a surprising reason: the rotatory strength integrated over all frequencies is equal to the sum of the Chern numbers of all the Fermi-surface pockets, which in turn must vanish for topological reasons.



HIGHLIGHT 11

Radiative cooling properties of Portlandite and Tobermorite: two cementitious minerals of great relevance in concrete science and technology

Jorge S. Dolado, Guido Goracci, Silvia Arrese-Igor, Andrés Ayuela, Angie Torres, Iñigo Liberal, Miguel Beruete, Juan J. Gaitero, Matteo Cagnoni, and Federica Cappelluti

ACS Applied Optical Materials

The capacity of concrete for daytime radiative cooling applications remains largely untapped. This study delves into the radiative properties of Portlandite and Tobermorite, two essential minerals in cementitious structures. Our findings provide substantial insights into the necessary composition and porosity of concrete to unlock its daytime radiative cooling capabilities.

Although concrete and cement-based materials are the most engineered materials employed by mankind, their potential for use in daytime radiative cooling applications has yet to be fully explored. Due to its complex

structure, which is composed of multiple phases and textural details, fine-tuning of concrete is impossible without first analyzing its most important ingredients.

In this context, researches of the MIRACLE's partnership have studied Portlandite ($\text{Ca}(\text{OH})_2$) and Tobermorite ($\text{Ca}_5\text{Si}_6\text{O}_{16}(\text{OH})_2 \cdot 4\text{H}_2\text{O}$), two minerals of great relevance in cement and concrete science and technology, and compared their radiative cooling properties to the ones of normal cement pastes.

This work has combined numerous computational methodologies (including force field atomistic simulations, Mie Theory, and Bruggeman homogenization schemes) with spectroscopic experiments (UV-Vis-NIR reflectance and IR emissivity measurements).

In essence, the work demonstrates that, in contrast to concrete (which is a strong infrared emitter but a poor sun reflector), both Portlandite and Tobermorite have very good sun reflectance (0.93 and 0.75 respectively)

and high emissivity within the Atmospheric Window (0.84 and 0.85 respectively). Besides the work has demonstrated that the emissivity of concrete can be tuned by playing with the porosity.

Overall, the results provide valuable insights into the optimization of concrete composition and porosity to achieve effective daytime radiative cooling.

**"Let's make NEW
«cool» concretes"**

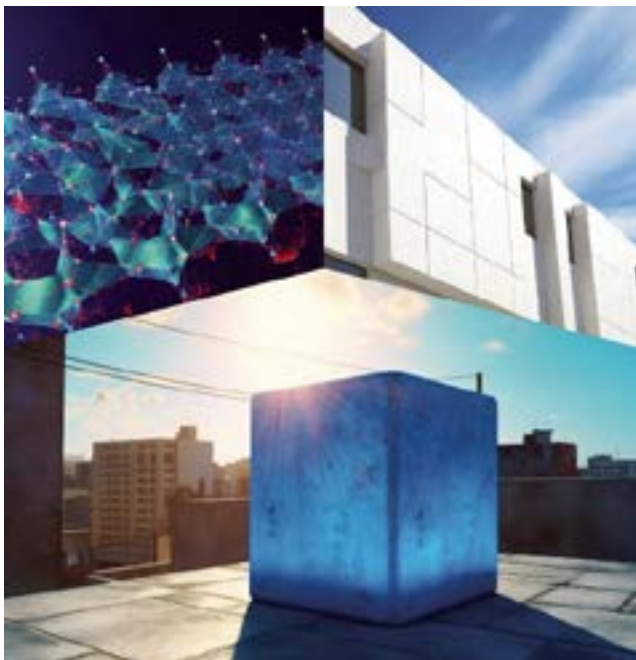


Figure: AI- image that illustrates an optimized "cool" concrete. This image has been chosen as cover of the journal.

HIGHLIGHT 12

Understanding the large shift photocurrent of WS₂ nanotubes: a comparative analysis with monolayers

Jyoti Krishna, Peio Garcia-Goiricelaya, Fernando de Juan, and Julen Ibañez-Azpiroz.

Physical Review B 108, 165418 (2023)

The bulk photovoltaic effect generates a dc current in acentric materials upon light absorption. Transition metal dichalcogenide nanotubes offer an ideal platform to study the effect, given the large light-absorption capabilities of the constituent materials in two-dimensions. This study analyzes the shift-current contribution to the bulk photovoltaic effect in WS₂ nanotubes using ab-initio calculations, and places the theoretical results in the context of recent experimental measurements.

Current solar-cells are based on the standard photovoltaic effect and employ so-called pn-junctions, namely interfaces between two different semiconductors that generate a built-in electric field that drives the photo-excited electrons. Interestingly, crystals that lack an inversion center in their crystalline structure exhibit a

distinctive effect, namely the bulk photovoltaic effect. In contrast to the standard effect in pn-junctions, the bulk photovoltaic effect is quadratic in the electric field of light and occurs in homogeneous crystals; therefore it needs no interfacing technique to be employed as a solar cell. In simple terms, this effect converts light into electricity intrinsically. Its implementation would open the door to solar-cells potentially exceeding current technologies, which can play an important role in coming years.

In this study, the researchers investigated a central contribution to the bulk photovoltaic effect, namely the shift photocurrent, in transition-metal dichalcogenide monolayers and nanotubes. The analysis is based on density functional theory in combination with the Wannier interpolation technique, and the results show that for a nanotube radii of practical interest $r > 60$ Å, the shift photoconductivity of a single-wall nanotube is well described by that of the monolayer. Additionally, the research team has quantified the shift photocurrent generated under realistic experimental conditions like device geometry and absorption capabilities, showing that a typical nanotube can generate a photocurrent of around 10 nA, while the monolayer only attains a maximum of 1 nA. This enhancement is mainly due to the larger conducting cross section of a nanotube in comparison to a monolayer.

"This study analyzes the shift-current contribution to the bulk photovoltaic effect in WS_2 nanotubes using ab-initio calculations, and places the theoretical results in the context of recent experimental measurements"

These findings suggest that the large nonlinear photocurrent measured recently in WS_2 nanotubes [Zhang *et al.*, Nature (London) 570, 349 (2019)] originates from the shift mechanism, making nanotubes a promising platform for solar energy extraction via the bulk photovoltaic effect.

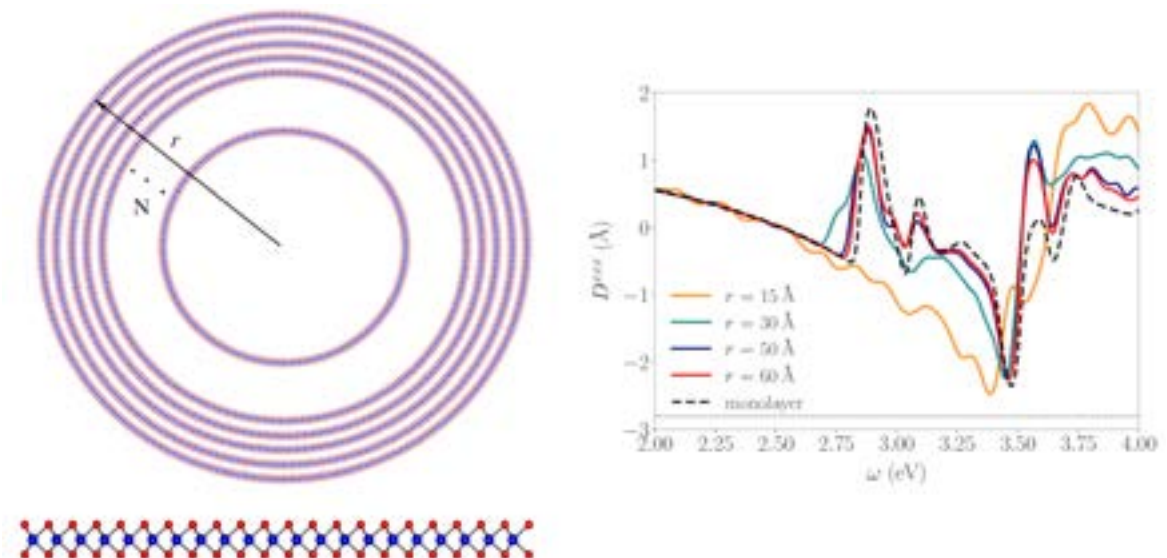


Figure: On the left, a multiwall zigzag nanotube of radius r composed of N layers and a two-dimensional hexagonal monolayer. On the right, the calculated shift distance tensor component xxx as a function of photon frequency for single-wall nanotubes with varying radii (r) and a monolayer. The nanotube result is seen to converge to the monolayer limit above $r > 60$ Å. The grey dashed line shows the average bond length of 2.8 Å between the ions in the monolayer.

HIGHLIGHT 13

Modifying the energy of collective molecular vibrations through optomechanical interaction

Lukas A. Jakob, William M. Deacon, yuan Zhang, Bart de Nijs, Elena Pavlenko, Shu Hu, Claudy Carnegie, Tomas Neuman, Ruben Esteban, Javier Aizpurua, and Jeremy J. Baumberg.

Nature Communications 14, 3291 (2023)

Visible photons can interact with molecular vibrations of much smaller energies through an inelastic scattering process. The strong field confinement induced by plasmonic resonances in metallic nanocavities can activate an intense optomechanical interaction, producing large energy shifts of collective molecular vibrations.

The resonant oscillation of atoms in molecules at well-defined energies, results in a set of vibrational modes in the THz to mid-infrared spectrum specific to each molecule, and serve to fingerprint a molecule for selective detection and characterization. With this purpose, Raman spectroscopy exploits the optomechanical interaction between molecular vibrations (the mechanical modes) and optical photons in a cavity at visible and near-infrared frequencies. In this process, photons exchange energy with vibrations of much smaller energy, resulting in the emergence of photons of slightly shifted energy (Figure inset).

The Raman signal is usually very weak, but the efficiency of the optomechanical interaction can be strongly boosted by placing the molecules near metallic nanostructures that support resonant collective oscillations of the free electrons of the metal, the so-called plasmonic modes, which confine the optical energy to extremely small volumes. This technique is called Surface-Enhanced Raman Spectroscopy (SERS) and is widely used for molecular characterization and sensing. In the last decade, a cavity quantum electrodynamics description based on quantum optomechanics has been developed to describe SERS..

In this work, the team of the “Theory of Nanophotonics” group at CFM and DIPIC, together with collaborators at Zhengzhou University, China, further developed the optomechanical description of SERS to calculate the Raman signal from many molecules situated in an extremely narrow gap, taking into account the full plasmonic response and plasmon-mediated vibration-vibration interactions. The results show that different collective vibrational modes are activated, and each of them experiences a different optomechanically-induced change of its energy and effective losses. These changes can be detected by a modification of the shape of the individual peaks in the Raman spectra, which split from a single Lorentzian spectral feature at

weak laser intensities into two peaks of different energy and width as the laser intensity is increased (Figure). Further, this prediction is supported by experimental measurements by collaborators in Cambridge University, United Kingdom. These results thus indicate that collective vibrational properties of molecules can be modified through an enhanced optomechanical interaction in plasmonic nanocavities.

"The optomechanical interaction between molecules and plasmonic cavities opens a new pathway to induce collective molecular vibrational modes and to control their energies by optical means"

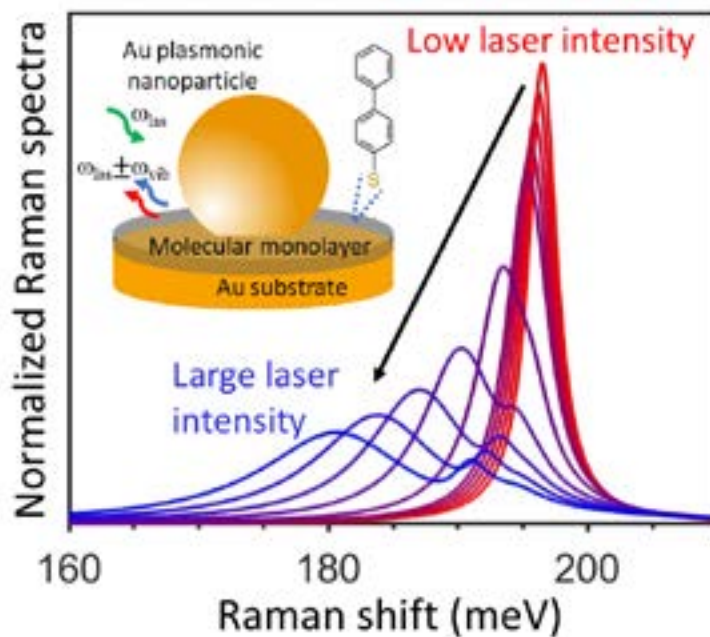


Figure: ω_{las} and ω_{vib} the frequency of the excitation light and of the molecular vibrations, respectively.

HIGHLIGHT 14

Thermoplasmonic self-oscillator based on gold nanoparticles

Stefano A. Mezzasalma, Joscha Kruse, Stefan Merkens, Eneko Lopez, Andreas Seifert, Roberto Morandotti, and Marek Grzelczak.

Advanced Materials 35, 2302987(2023)

Self-oscillation is the generation of a periodic change in a system by a non-periodic power source. The ability of a self-oscillator to maintain its frequency enables the conversion of a steady input into a usable oscillating output, a feature present in many biological systems (e.g., neuron firing, heart beating) and synthetic materials (e.g., hydrogels or elastomers).

An international squad of researchers from Spain, Canada, and Croatia, led by Marek Grzelczak (CFM), proposed a new type of self-oscillator. They have introduced a theoretical model, backed by experiments, that revolves around gold nanoparticles that spontaneously come together in clusters. The team observed that when these nanoparticles cluster, they become efficient local heaters due to their strong absorption of light (Figure).

This leads to an interesting chain of events, where the heated clusters not only disperse again but eventually showed rhythmical clustering and dispersing under constant light illumination. The developed theory predicts that the surface temperature of thermoplasmonic nanoparticles and the number density of their clusters jointly oscillate at frequencies ranging from infrasonic to acoustic values. What's more, as the researchers delve deeper into the nonlinear aspects, they uncover a whole new world of complexity, with the emergence of dynamic attractors that connect thermoplasmonics to nonlinearity and chaos.

Essentially, this research offers a glimpse into the future of soft robotics and self-propelled machinery down to the scale of nanoparticles, enabling engineering tiny systems that can move on their own, from precise and predictable motions to whimsical and dynamic performances.

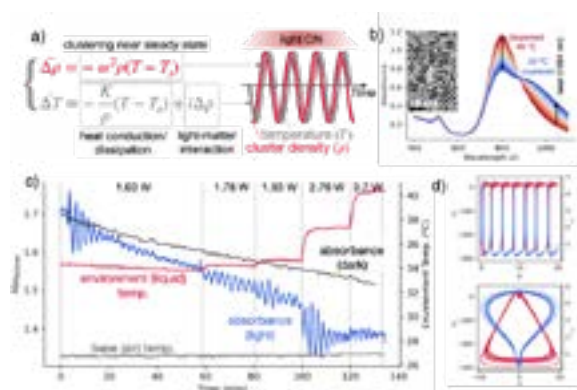


Figure: Thermoplasmonic self-oscillator. A) theoretical model predicting oscillatory clustering of gold nanoparticles. B) Reversibly clustering gold nanorods upon temperature drop. C) oscillatory clustering under different light power density. D) Theoretical prediction of a dynamic system exhibiting attractor-like behaviour.

HIGHLIGHT 15

Novel Sol-Gel route to prepare Eu^{3+} -doped 80SiO_2 - 20NaGdF_4 oxyfluoride Glass-Ceramic for photonic device applications

María Eugenia Cruz, Thi Ngoc Lam Tran, Alessandro Chiasera, Alicia Durán, Joaquín Fernandez, Rolindes Balda, and Yolanda Castro.

Nanomaterials 2023, 13, 940

In this work, oxyfluoride glass ceramics with molar composition 80SiO_2 - $20(1.5\text{Eu}^{3+}:\text{NaGdF}_4)$ were prepared by sol-gel following the "pre-crystallized nanoparticles route" with promising optical results. Moreover, Eu^{3+} ion was selected as dopant due to its excellent properties as local probe, providing important information on the environment structure where it is located.

The development of transparent glass-ceramics (GCs) has drawn the attention of numerous researchers due to their important optical applications in light-emitting diodes, solar cells, sensing or in biomedical materials. Particularly, when fluoride nanocrystals smaller than 40 nm are dispersed in an oxide glass matrix, the resulting materials are transparent GCs, called oxyfluoride glass-ceramics (OxGCs), which have attractive properties. Among fluoride nanocrystals, those with formula ALnF_4 (where A is an alkaline element and Ln a lanthanide), have become more attractive in comparison to other fluorides due to their lowest phonon ener-

gies and wide band gap (9-10eV). 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 also allows the final crystal fraction to be controlled by avoiding fluorine loss, which occurs at high temperature during melting quenching, 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), OxGCs with molar composition 80SiO_2 - $20(1.5\text{Eu}^{3+}:\text{NaGdF}_4)$ were prepared by sol-gel following the "pre-crystallized nanoparticles route" with promising optical results. The preparation of 1.5 mol % Eu^{3+} -doped NaGdF_4 nanoparticles was optimized and characterized by XRD, FTIR and HRTEM (Figure 1). The structural characterization of 80SiO_2 - $20(1.5\text{Eu}^{3+}:\text{NaGdF}_4)$ OxGCs prepared from these nanoparticles' suspension revealed the presence of hexagonal and orthorhombic NaGdF_4 crystalline phases. The optical properties of both nanoparticles' phases and the related OxGCs were studied by measuring the emission and excitation spectra together with the lifetimes of the 5D_0 state. The emission spectra obtained by exciting the Eu^{3+} - O_2 - charge transfer band showed similar features in both cases corresponding the higher emission intensity to the $^5\text{D}_0 \rightarrow ^7\text{F}_2$ transition that indicates a

non-centrosymmetric site for Eu^{3+} ions. Moreover, time resolved fluorescence line-narrowed emission spectra obtained under selective excitation in the ${}^7\text{F}_0 \rightarrow {}^5\text{D}_0$ transition at 9 K allow to identify two distinguishable sites for Eu^{3+} ions in the OxGCs powders with C2v and C3

symmetries, which are compatible with the observed hexagonal and orthorhombic phases detected in the XRD diffraction patterns. The results show that this processing method is promising to prepare transparent OxGCs coatings for photonic applications.

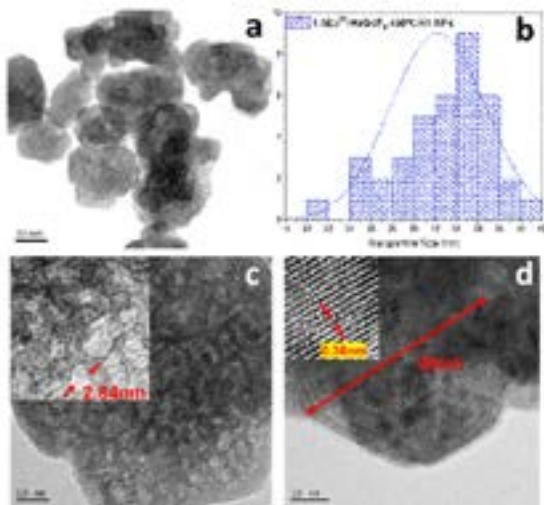


Figure 1: HR TEM images of (a) $1.5\text{Eu}^{3+}:\text{NaGdF}_4$ NPs heat-treated at 450°C for 5 h. (b) The corresponding nanoparticle size distribution taken from the image on “a”, (c) Amplification of the area selected in “a” with the porous size measurement. (d) Amplification of the area selected in “a” with the lattice distance measurement.

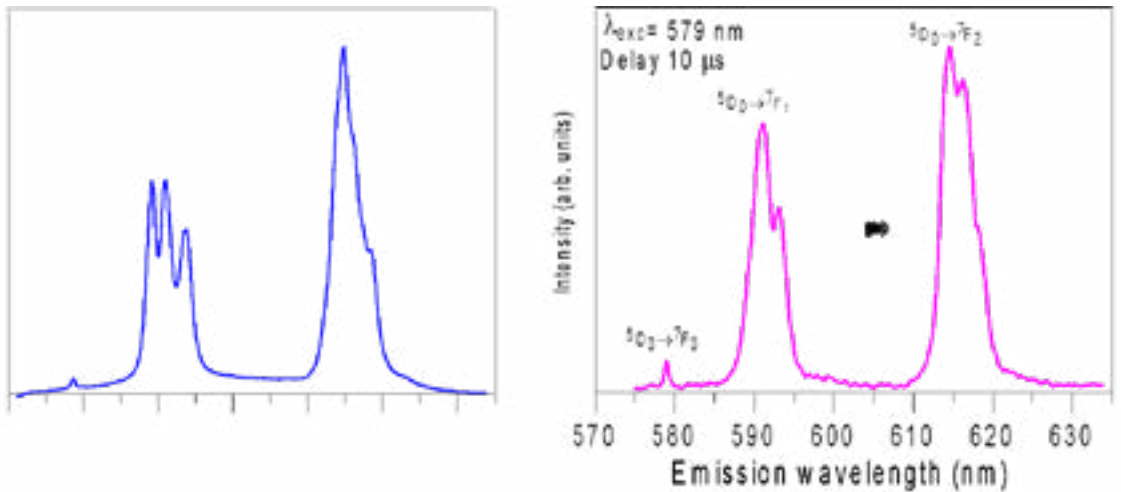


Figure 2: Time-resolved fluorescence line-narrowed emission spectra of the ${}^5\text{D}_0 \rightarrow {}^7\text{F}_{0,1,2}$ transitions of Eu^{3+} ions measured at 9 K at a time delay of 10 μs after the laser pulse under an excitation at (a) 578.6 nm and (b) 579 nm, respectively, for the $80\text{SiO}_2\text{-}20(1.5\text{Eu}^{3+}:\text{NaGdF}_4)$ powders heat-treated at 450°C for 5 h.

HIGHLIGHT 16

Metamorphosis of a commodity plastic like PVC to efficient catalytic single-chain nanoparticles

Agustín Blázquez Martín, Ester Verde Sesto, Arantxa Arbe and José A. Pomposo.

Angewandte Chemie International Edition 62, e202313502 (2023)

In addition to recycling, waste valorization by converting polymeric waste materials into more useful products is attracting significant interest to mitigate plastic pollution issues. In this sense, polyvinyl chloride (PVC) is the 3rd most widely produced synthetic polymer in the world.

Mechanical recycling of rigid PVC from the construction and building sector (e.g., windows, pipes) is currently the main relevant recycling process in the EU for post-consumer PVC waste. Recycling or valorization of flexible PVC waste from e.g. packaging, automotive and medical sectors is complicated by the difficulty to handle banned plasticizers (e.g., bis(2-ethylhexyl)

phthalate) -still entering recycling streams- after isolation of neat PVC from flexible PVC waste. Currently, significant effort is devoted by many research groups on breaking PVC down to useful products.

This work reports on a complementary concept of polymeric waste valorization (upcycling) by metamorphosis of a commodity plastic of common use in daily life like polyvinyl chloride (PVC) to “valorized” PVC single-chain nanoparticles (vPVC-SCNPs) (**Figure, panel a and b**). Until now, SCNPs were always synthesized from specialty polymeric precursors and not from waste of commodity plastics. The full valorization process (PVC isolation, PVC azidation, vPVC-SCNPs

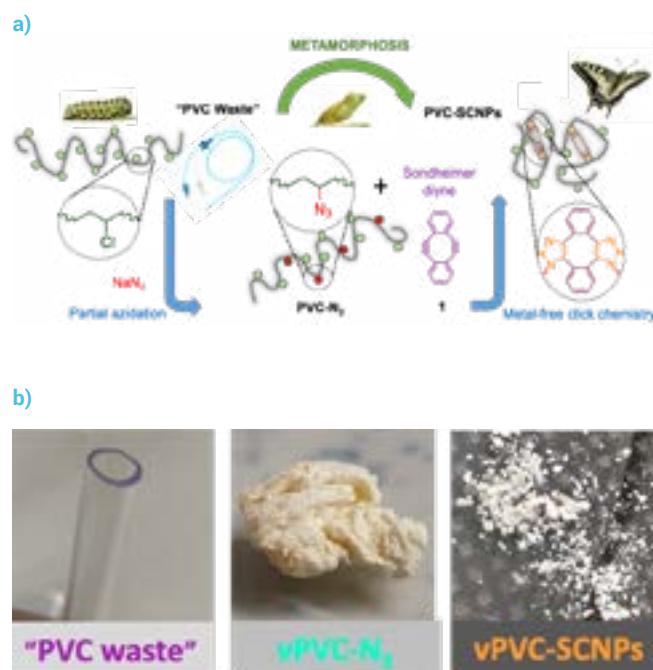


Figure: (a) Illustration of the metamorphosis of “PVC waste” to valorized PVC single-chain nanoparticles (vPVC-SCNPs). (b) The valorization process by starting with an out-of-use PVC hose to give vPVC-SCNPs.

synthesis) can be run in a green, dipolar aprotic solvent like N-butylpyrrolidinone (NBP) and involving, when required, a simple mixture of ethanol and water (1/1 vol.) as non-solvent. The metamorphosis process when carried out via metal-free click chemistry by means of the Sonheimer diyne as intra-chain cross-linker plus a specific end-capping procedure with benzyl azide leads to well-defined, uniform vPVC-SCNPs that are stable during storage in the solid state for months.

These nanoparticles when loaded with 7.3 mol % of Cu(II) ions -to give vPVC-SCNPs/Cu(II)- become an efficient and recyclable catalyst in the solvent-free ho-

mocoupling reaction of polar alkynes. They show enzyme-mimetic behavior in the oxidation of 3,5-di-tert-butylcatechol to 3,5-di-tert-butyl-o-quinone (**Figure, panel c**) as well as very high turnover frequency (moles of product per mole of catalyst per unit of time, TOF) in the peroxidative oxidation of styrene to benzaldehyde. We envision the use of vPVC-SCNPs/Cu(II) as efficient catalyst in other Cu(II)-catalyzed organic transformations like cyclopropanation, Chan–Lam coupling or the Henry reaction, among others. Notably, this new concept is amenable for the valorization of other commodity plastics in which it is feasible to install azide functional groups along their linear polymer chains.

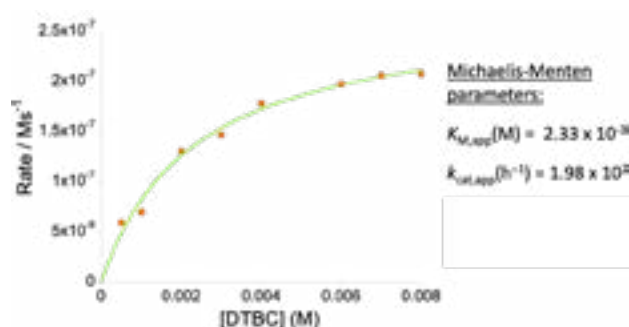


Figure c: Metalloenzyme-mimetic properties of vPVC-SCNPs loaded with 7.3 mol% of Cu(II) ions in the oxidation of 3,5-di-tert-butylcatechol to 3,5-di-tert-butyl-o-quinone.

HIGHLIGHT 17

Microscopic evidence for the topological transition in model vitrimers

Arantxa Arbe, Angel Alegria, Juan Colmenero, Saibal Bhaumik, Konstantinos Ntetsikas, and Nikos Hadjichristidis.

ACS Macro Letters 12, 1595 (2023)

Vitrimers consist of permanent networks containing dynamic bonds that allow the topology of the network to change, keeping always constant number of cross-links. In addition to the glass transition, vitrimers undergo a topological transition from viscoelastic liquid to viscoelastic solid behaviour when the network rearrangements facilitated by dynamic bond exchange reactions freeze. The microscopic observation of the topological transition is elusive.

Model polyisoprene vitrimers were investigated. In these dynamic networks nanophase separation of polymer and reactive groups leads to the emergence of a relevant length scale characteristic for the network structure, as observed by SAXS. Clusters of linkers separated by an average distance D give rise to a clear peak in the structure factor, while the correlations between adjacent chains emerge as a peak at much higher Q -values, revealing the inter-chain distance d (Figure 1). Exploiting the scattering sensitivity to structural features at different length scales, makes possible to determine how dynamical and topological arrests affect correlations at segmental and network levels. This was realized by following the thermal evolution of inter-cluster and inter-chain correlations ('microscopic dilatometry'). At the inter-chain level, chains expand obeying the same expansion coefficient throughout the entire viscoelastic region, i.e., both in

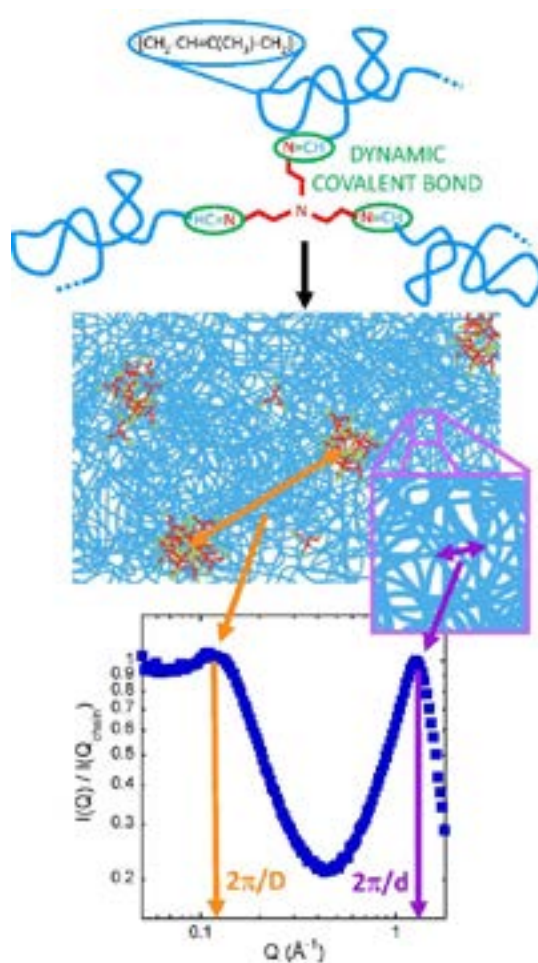


Figure 1: Upper panel: Schematic representation of the vitrimer. Central panel: Drawing of the nano-segregated structure suggested by SAXS. Lower panel: SAXS results corresponding to the lowest molecular weight investigated.

the elastomeric regime and in the liquid regime (Figure 2a). The onset of liquid-like behaviour is only apparent at the mesoscale, where the scattering reveals features related to the reorganization of the network triggered by bond exchange events (Figure 2b). This is manifested by different expansion of the clusters including the dynamic bonds below and above a temperature identified as the "microscopic" topological transition temperature T_v . Proper thermal (aging-like) protocols were proposed, and revealed signatures of the 'microscopic' topological transition also by a 'macroscopic' technique such as the Differential Scanning Calorimetry (DSC) (Figure 2c), opening the door to identify this important transition temperature also by a standard technique.

"Scattering sensitivity to structural features at different length scales allows determining how dynamical and topological arrests affect correlations at segmental and network levels, revealing thereby the topological transition"

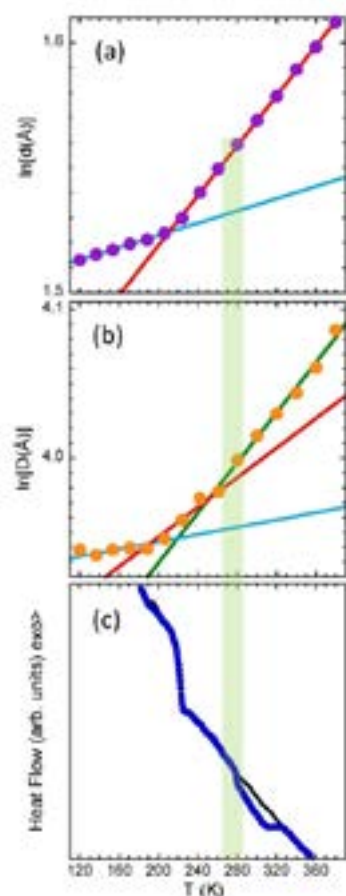


Figure 2: Temperature dependence of the natural logarithm of the average interchain distance, $\ln(d)$ (a) the average intercluster distance $\ln(D)$ (b) and heat flow (c). Calorimetric results were obtained on heating after fast cooling (black lines) and after slow cooling (blue points). Shadowed red area indicates the location of T_v .

HIGHLIGHT 18

Dual crosslinking of low-methoxyl pectin by calcium and europium for the simultaneous removal of pharmaceuticals and divalent heavy metals

Javier Martínez-Sabando, Francesco Coin, Juan Carlos Raposo, Aitor Larrañaga, Jorge H. Melillo, Silvana Cerveny.

Chemical Engineering Journal 475, 146162 (2023)

Patent inventors: J. Martinez Sabando, F. Coin, G.A. Schwartz and S. Cerveny.

Composition for removing pharmaceuticals and heavy metals from polluted water (EU Patent EP22383090.2)

Water is fundamental to our society's progress and economic development and essential for human survival, agriculture, healthcare, industry, and safety. Furthermore, water is intrinsically linked to the financial well-being of our communities, and currently, there is no alternative to water on the surface of our planet. However, emerging contaminants, a group of unregulated pollutants such as pharmaceuticals, heavy metals, pesticides, and personal care products, are being detected in water sources more frequently than ever, and it is necessary to take action urgently. These contaminants pose severe environmental and human health risks and are difficult and expensive to remove.

In this study (collaboration between CFM, DIPC, MPC, and UPV/EHU) has developed an adsorbent based on pectin (a recyclable, biodegradable, and cost-effective

material), which is highly effective for the simultaneous removal of both heavy metals and pharmaceutical products from water. The novel approach includes the gelation of pectin by crosslinking it with different agents: calcium, europium, and their combination. The reticulated pectin structures exhibited significant structural differences depending on the type of crosslinking agent used, affecting adsorption capacity. Specifically, calcium cations partially formed a crystalline "egg-box" structure, whereas europium cations produced an amorphous network without crystalline regions. The dual-crosslinking system resulted in an intermediate network with crystalline and amorphous regions.

The findings show that dual-cross-linked pectin is a highly effective adsorbent for the simultaneous

removal of heavy metals and pharmaceutical products. The material can capture over 99% of metals and more than 70% of drugs. This novel approach of crosslinking pectin with multiple agents has the potential to significantly enhance its remediation capacity, offering a promising solution for the simultaneous removal of numerous pollutants from water.

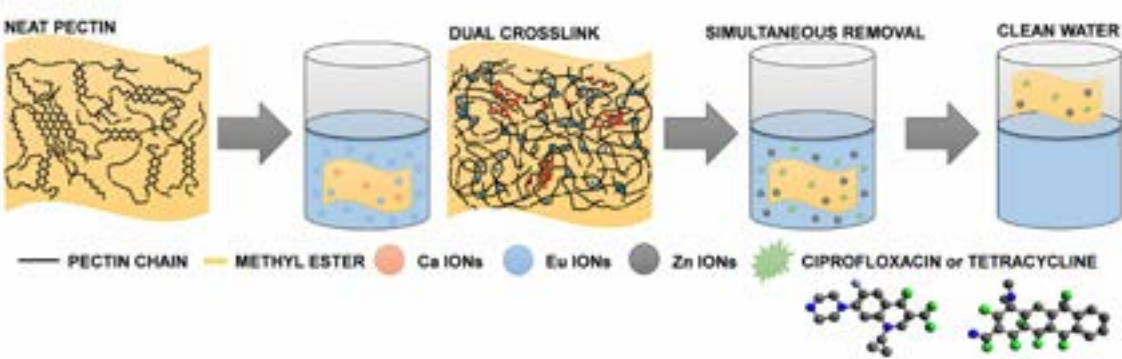


Figure: Schematic representation of water remediation using pectin-based adsorbents.

HIGHLIGHT 19

Size-dependent vitrification in metallic glasses

Valerio Di Lisio, Isabella Gallino, Sascha Sebastian Riegler, Maximilian Frey, Nico Neuber, Golden Kumar, Jan Schroers, Ralf Busch and Daniele Cangialosi.

Nature Communications 14, 4698 (2023)

Metallic glasses are materials of extraordinary importance due to their superior mechanical properties and corrosion resistance. A well-known and widely investigated aspect, which deeply impacts the metallic glass final properties, is that their thermodynamic state depends on the processing conditions employed to produce them.

Hitherto the way reducing the sample size affects the glass thermodynamic state of the metallic glass and the implications on their final properties remains much less investigated. This work presents a study on the way vitrification – the transformation to a glass on cooling the liquid – takes place in two metal alloys based on gold and platinum, depending on certain conditions. More specifically, the sample size and applied cooling rate are varied using state-of-the-art fast scanning calorimetry that permits achieving heating/cooling rates as large as 40000 K/s. The key result of the study is that reducing the sample size to the micrometer scale allows conveying the glass to low energy/high density states, as parametrized by the fictive temperature, T_f , of the glass. While this effect is minimized in glasses cooled at high rates, cooling at rates of several K/s or lower allows attaining reduction in T_f of as low as 40 K below the glass transition temperature of the metal alloy for the smallest samples, a reduction that would require geological time scales in a bulk glass. Applying the free volume holes diffusion model allows capturing

this phenomenology – where enthalpy reduction / density increase is assisted by release of free volume to the free interface.

These findings have profound implications on both technological and fundamental perspectives. They show how low energy/high density metallic glasses can be produced on time scales of seconds simply reducing the sample size. In this way, they open the door to reaching thermodynamic states otherwise unattainable on conventional bulk glasses in time scales accessible to the human being, thereby allowing exploring the fate of the thermodynamic state of a glass deep in the energy landscape. Specifically, the long-standing issue of the existence of a true thermodynamic transformation into the so-called “ideal glass”, recently unveiled in polymeric glasses, can be explored in metallic glasses too, involving times scales amenable to the experimental practice.

“Fast scanning calorimetry allows detecting a hitherto unknown sample size effect on metallic glasses vitrification”

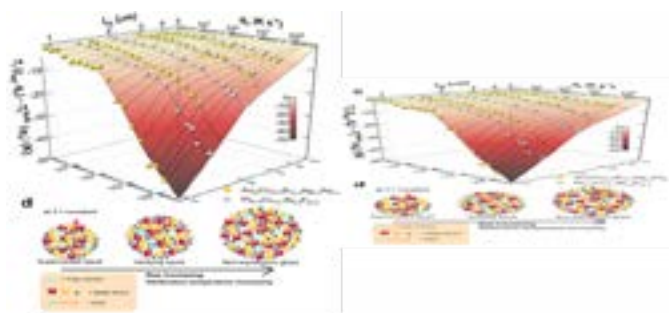


Figure: (Left) T_f reduction with respect to the bulk as a function of cooling rate, q_c , and sample size, L_{eq} , for gold and platinum based metallic glasses and (Right) schematic plot of the free volume holes diffusion model.

HIGHLIGHT 20

Quantum tunneling rotors unravel gas-uptake pathways in metal-organic frameworks

Kirill Titov, Matthew R. Ryder, Aran Lamaire, Zhixin Zeng, Abhijeet K. Chaudhari, James Taylor, E.M. Madhi, Sven M.J. Rogge, Sanghamitra Mukhopadhyay, Svemir Rudić, Veronique Van Speybroeck, Felix Fernandez-Alonso, and Jin-Chong Tang.

Physical Review Materials 7, 073402 (2023)

Metal-organic frameworks can store sizable quantities of gaseous species, with immediate applications in the sequestration of greenhouse or flue-gas emissions from industrial processes. By virtue of their carbon-based nature, their inherent flexibility also leads to novel sorption mechanisms, which still defy a robust understanding at the atomic and molecular levels.

To address the above challenge, this work has capitalized from recent developments in simultaneous neutron diffraction and spectroscopy, to study in-situ and at an unprecedented level of detail the adsorption of host species in the zeolitic imidazolate framework ZIF-8. Extensive first-principles calculations were also deployed to interpret the experimental results in a quantitative manner. The nanopores in ZIF-8 are decorated with an ordered ensemble of methyl (-CH₃) functional groups where the three protons become indistinguishable via quantum tunneling (Figure). This

phenomenon gives rise to a well-defined energy-level structure uniquely sensitive to subtle changes to the potential energy landscape inside the pore in the absence and presence of guest species. The bottom panel in the figure shows experimental results for the case of argon. With the neutron data, we can dissect the adsorption isotherm into the filling of distinct sites. The trends at low pressures show differences relative to higher-pressure conditions, particularly in terms of the inability in the former case to access the four-membered rings within the porous structure. In both situations, other adsorption sites on either side of these tight rings are accessible and occupied when a sufficient amount of gas is supplied. Unveiling this behavior with a genuinely quantum probe is key to understanding the gas-uptake response: the steps seen in the adsorption isotherms, tunneling spectra, and diffraction patterns only occur after the two most readily accessible sites have been filled in a sequential manner. Structurally, this process requires a rotation of the organic linker within the framework, to make other sites accessible via a dynamic ‘gate-opening’ mechanism. Progressively, it also leads to a ‘gate-blocked’ structure where the linkers are no longer able to rotate into a ‘gate-closed’ position owing to the presence of the adsorbate. These effects are accompanied by changes to the long-range order of the framework (lower-right

panel of the figure). In addition to these much-needed physical insights, this study also offers a glimpse at the yet-to-be-tapped scientific potential for materials research of the European Spallation Source, soon to become operational in Lund, Sweden.

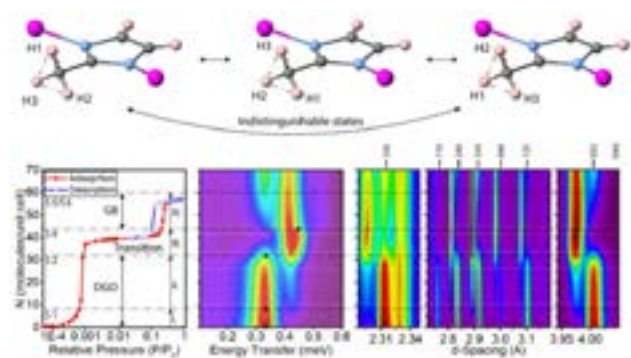


Figure: (Top panel) Schematic diagram of the methyl-group motif in ZIF-8, highlighting the three indistinguishable protons via rotation about the carbon-carbon axis. (Bottom panel) Experimental results for the case of argon – from left to right: adsorption-desorption isotherms; methyl-tunneling inelastic neutron-scattering spectra; and neutron diffraction.

"Quantum tunneling reveals the microscopic mechanisms underpinning the uptake of gaseous species in metal-organic frameworks"

FACILITIES & EXTERNAL SERVICES

CFM infrastructure has been envisioned to characterize nanoscale materials with high sensitivity. Thus, the CFM headquarters building 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 were launched progressively, completing 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

LIQUID HELIUM RECOVERY AND SUPPLY PLANT FOR CRYOGENIC EXPERIMENTAL SYSTEMS

Due to the scarcity of liquid helium, its high cost and the strong dependence on its continuous supply by external suppliers, the performance of the experimental equipment in the CFM and its operability were compromised. Put into use in 2022, the Helium recovery and supply plant has proven a permanent solution to this problem, providing the CFM and its researchers with a common benefit facility that reduces research costs.

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

CHEMICAL PHYSICS OF COMPLEX MATERIALS

CRYOGENIC SYSTEM FOR PHYSICAL CHARACTERIZATION OF DEVICES

Dilution refrigerator Oxford Proteox MX 500 with a base temperature of 7mK and uniaxial magnetic fields of up to 7 T. This fridge allows for experimental investigation of quantum phenomena in superconductors or in the new topological phases of semiconductors. Custom copper cold finger and printed circuit board sample holders were designed and fabricated to handle the samples for the DC transport measurements. Cryogenic filters and a modern nano Volt/Ampere meters complement the setup electronics reaching the sensitivity level suitable for characterization of superconducting and semiconducting qubits.

HIGH RESOLUTION ANGLE RESOLVED PHOTOEMISSION

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.

FACILITIES

SURFACE CHEMICAL-PHYSICS

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 Microscope (STM) (with the possibility to use in Atomic Force Microscope (AFM) mode). The chamber has two samples preparation chambers, with the required Molecular Beam Epitaxy (MBE) and sample preparation tools.

SURFACE MAGNETISM

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 MICROSCOPES

Our institution currently hosts two Scanning Tunneling Microscopes (STMs). An Atomic Force Microscopy (AFM) - STM operable at 1K for characterization of materials at atomic scale, as well as a continuous flow cryostat LHe/LN2 low temperature functioning at liquid helium/liquid nitrogen temperature to study electrical properties of molecules and atoms on surfaces and growth of chemical synthesis.

ELECTRONIC PROPERTIES AT THE NANOSCALE

CERAMICS AND CEMENT-BASED MATERIALS

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).

FACILITIES

ULTRAFAST SPECTROSCOPY LAB

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

NANOPHOTONICS 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 photo luminescence 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
- 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

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).

FACILITIES

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)
- 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 nanositioners, for cooling down nanostructures and nanoparticles to cryogenic temperatures (attoDRY 100 model from Attocube)
- A set of spatial light modulators (from Cambridge Correlators), polarizers (from Thorlabs and Standa) and Single Photon Counting Modules (SPCM, APDs SPCM-AQ4C model from Excelitas), for analyzing the photons interacting with nanostructures at cryogenic temperatures
- Microwave generators and amplifiers (SMB100A model from Rohde & Schwartz), for addressing the electronic states of Nitrogen Vacancy centers in diamond

POLYMERS AND SOFT MATTER

DIELECTRIC SPECTROSCOPY LAB

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

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

MICROSCOPY LAB

The “Microscopy” laboratory allows materials’ structural characterization by means of:

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

FACILITIES

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
- Viscosimeters: EMS-1000 and Malvern SV-10 Vibro
- Surface tension meter: Contact Angle meter OCA 15 EC DataPhysics Instruments GmbH
- Liquid/solution density meter: ANTON PAAR, DMA 4500 M model
- UV-VIS spectrometer: Agilent 8453A with Peltier thermostated cell holder, T-controller 89090A
- Close vessel microwave assisted reactor: CEM Discover SP System (200-550K, 0-27 bar)

THERMAL CHARACTERIZATION LAB

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

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

RHEOLOGICAL CHARACTERIZATION LAB

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

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

ABSORPTION SPECTROSCOPY TECHNIQUES LAB

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

- For the molecular spectroscopy in the infrared (IR) domain: FT-IR - JASCO 6300 (130-400K)
- For the molecular spectroscopy in the terahertz (THz) domain: TPS SPECTRA 3000, TeraView
- Raman scattering: FT-RAMAN, JASCO RFT-600

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.

FACILITIES

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 six 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.
- LeChuck cluster designed for Quantum ESPRESSO calculations and composed of 20 computing nodes with two AMD Milan 7443 processors (48 cores), 128GB and 1024GB of memory, and 54TB of shared storage, giving a total of 5.2TB of memory and 888 cores.
- Tanes 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 AMD Milan 7443 processors (48 cores), 256 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 3.3TB of memory.

These six 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 scientific computing workshops and tutorials.



EXTERNAL SERVICES

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 CFM qualified researchers and technicians at CFM's facilities, for researchers and technologists from different research fields and businesses. The CFM external services that can be commissioned are as follows:

HELIUM RECOVERY AND LIQUEFACTION SERVICE

This service offers liquid helium for ultra-low temperature experiments on a price per liter bases. Helium used in the CFM main building is retrieved through a recovery system collecting the evaporated helium released from the equipment with open helium cryostats located in the laboratories. It is subsequently liquefied again in our outdoors helium liquification plant.

SURFACE MAGNETISM ANALYSIS

The laboratory hosts equipment for surface characterization of samples by means of a homemade Magneto Optic Kerr Effect (MOKE, 15-300 K, 0.1 Tesla) and Scanning 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).

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.

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

76%

Published in the
Framework of International
Collaborations

211

ISI
Publications

84%

Open Access

89%

Q1

40%

D1

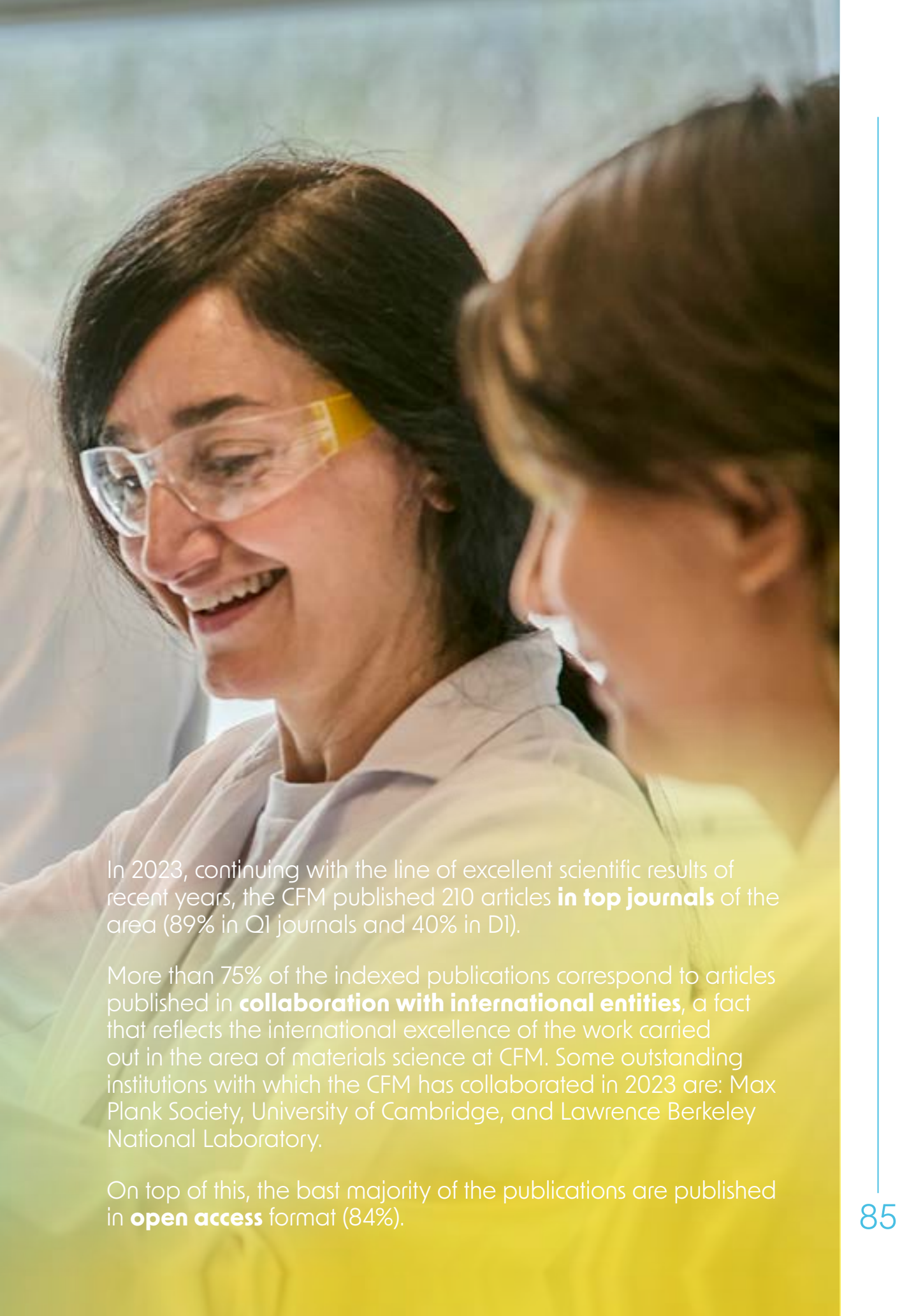
H-Index

161

ISI Web of Science citations

15 220* in 2023

*As of April 2024

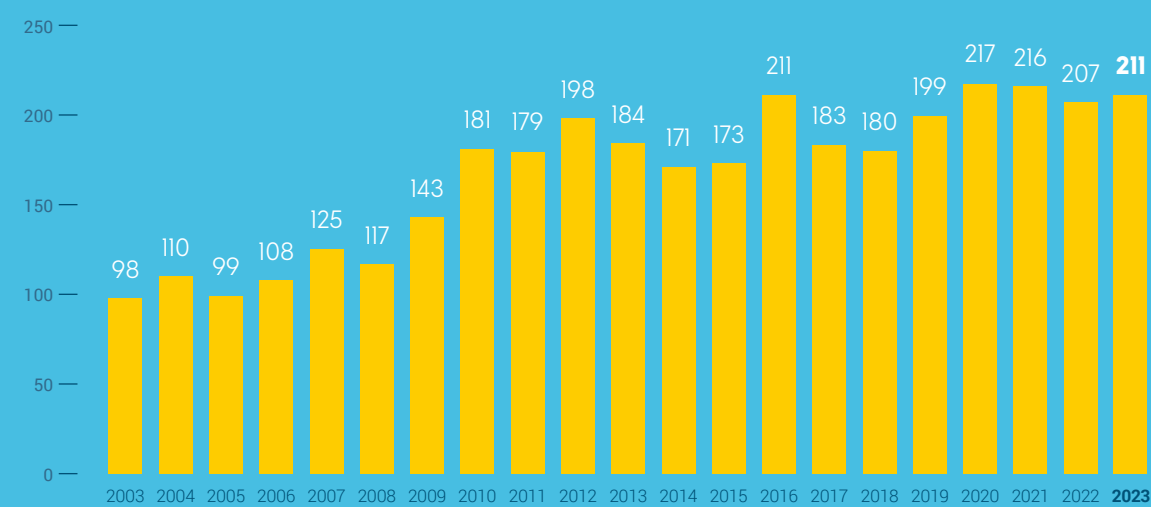


In 2023, continuing with the line of excellent scientific results of recent years, the CFM published 210 articles **in top journals** of the area (89% in Q1 journals and 40% in D1).

More than 75% of the indexed publications correspond to articles published in **collaboration with international entities**, a fact that reflects the international excellence of the work carried out in the area of materials science at CFM. Some outstanding institutions with which the CFM has collaborated in 2023 are: Max Plank Society, University of Cambridge, and Lawrence Berkeley National Laboratory.

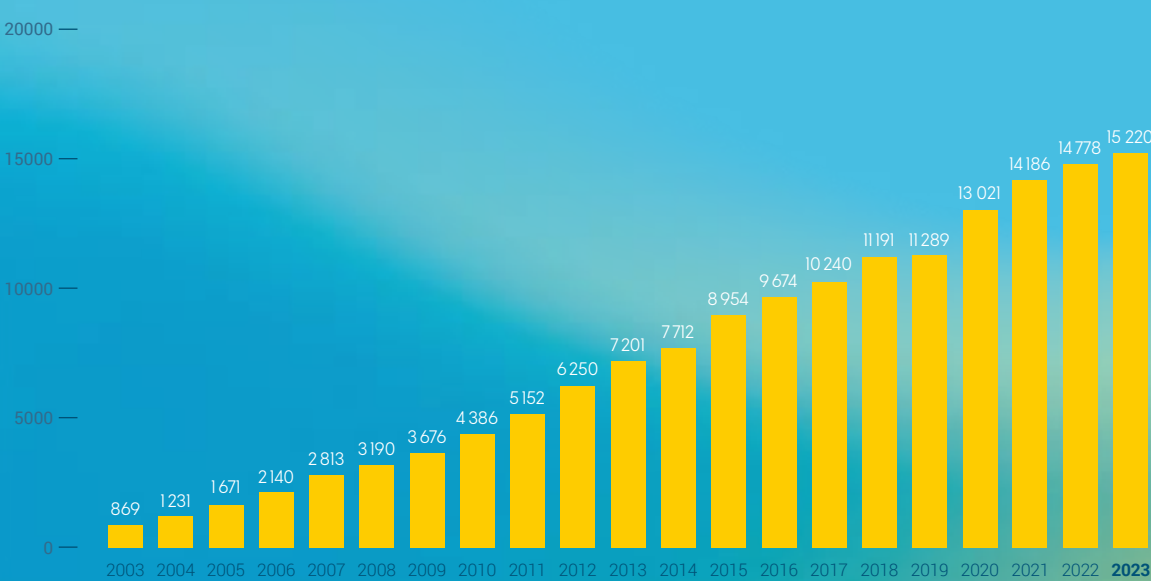
On top of this, the vast majority of the publications are published in **open access** format (84%).

PUBLICATIONS



Evolution of the publications of CFM over the years.
Total number of ISI Publications since 1999 as of April 2024: 3749

CITATIONS



Evolution of the citations of CFM over the years.
Total number of citations since 1999 as of April 2024: 155 895
H index (April 2024): 161

Total number of top publications:

61

JOURNAL	N° OF ARTICLES	IMPACT FACTOR
Science	2	59
Nature Materials	1	58,3
Advanced Materials	1	45,5
Angewandte Chemie	3	26,3
Journal of the American Chemical Society	2	25,7
ACS Nano	5	25,4
Nature Communications	11	24,9
Materials Horizons	1	22,2
Chemical Engineering Journal	2	21,5
ACS Catalysis	1	20,6
Science Advances	1	20,4
PNAS	1	19,2
Physical Review Letters	2	17
Progress in Photovoltaics	1	16,9
Chemistry of Materials	2	15,9
Journal of Colloid and Interface Science	4	15,5
Optical Materials	2	14,8
Nanoscale	6	13,6
ACS Photonics	3	12,7
NPJ 2D Materials and Applications	2	12,5
ACS Macro Letters	3	11,7
Materials Today Physics	1	11,7
Nanophotonics	1	11,3
Journal of Alloys and Compounds	3	10,9

PUBLICATIONS

- 1 Enhanced vacuum ultraviolet photoemission from graphene nanoribbons**
 Corso M, Lobo-Checa J, Weber AP, Piquero-Zulaica I, El-Fattah ZMA, Le Fevre P, Ortega JE, and Krasovskii E.
 2D Materials 11, 015008 (2023)
- 2 Radiative Cooling Properties of Portlandite and Tobermorite: Two Cementitious Minerals of Great Relevance in Concrete Science and Technology**
 Sanchez Dolado J, Goracci G, Arrese-Igor S, Ayuela A, Torres A, Liberal I, Beruete M, Gaitero JJ, Cagnoni M, and Cappelluti F.
 ACS Applied Optical Materials - Special Issue (2023)
- 3 Temperature and pH stimuli-responsive system delivers location-specific antimicrobial activity with natural products**
 Morris G, Goodman S, Bellido IS, Milanese C, Girella A, Pallavicini P, Taglietti A, Gaboardi M, Jäckel F, Fernandez YAD, and Raval R.
 ACS Applied Bio Materials 7, 131 (2023)
- 4 Highly durable nanoporous Cu₂-x S films for efficient hydrogen evolution electrocatalysis under mild pH conditions**
 Fernandez-Climent R, Redondo J, Garcia-Tecedor M, Spadaro MC, Li JN, Chartrand D, Schiller F, Pazos J, Hurtado MF, O'shea VD, Kornienko N, Arbiol J, Barja S, Mesa CA, and Gimenez S.
 ACS Catalysis 13, 10457 (2023)
- 5 Microscopic evidence for the topological transition in model vitrimers**
 Arbe A, Alegria A, Colmenero J, Bhaumik S, Ntetsikas K, and Hadjichristidis N.
 ACS Macro Letters 12, 1595 (2023)
- 6 Molecular mobility of polymers at the melting transition**
 Wang B, Sanviti M, Alegria A, and Napolitano S.
 ACS Macro Letters 12, 389 (2023)
- 7 Synthesis and characterization of a luminescent cyclic poly(ethylene oxide)-polypyridyl ruthenium complex**
 Aboudzadeh MA, Rodriguez-Fanjul V, Terenzi A, de San Roman EG, Miranda JI, Pizarro AM, Salassa L, and Barroso-Bujans F.
 ACS Macro Letters 12, 999 (2023)
- 8 Large orbital moment of two coupled spin-half Co ions in a complex on gold**
 Li C, Robles R, Lorente N, Mahatha SK, Rohlf S, Rosnagel K, Barla A, Sorokin BV, Rusponi S, Ohresser P, Realista S, Martinho PN, Jasper-Toennies T, Weismann A, Berndt R, and Gruber M.
 ACS Nano 17, 10608 (2023)
- 9 Controlling the spin states of FeTBrPP on Au(111)**
 Meng XZ, Moller J, Mansouri M, Sanchez-Portal D, Garcia-Lekue A, Weismann A, Li C, Herges R, and Berndt R.
 ACS Nano 17, 1268 (2023)
- 10 Self-enhancement of water electrolysis by electrolyte-poled ferroelectric catalyst**
 Li FS, Fang YW, Wu YT, Wu SW, Ho SZ, Chen CY, Chiang CY, Chen YC, and Liu HJ.
 ACS Nano 17, 16274 (2023)

PUBLICATIONS

- 11 Enhanced neuron growth and electrical activity by a supramolecular netrin-1 mimetic nanofiber**
Smith CS, Alvarez Z, Qiu RM, Sasselli IR, Clemons T, Ortega JA, Vilela-Picos M, Wellman H, Kiskinis E, and Stupp SI.
ACS Nano 17, 19887 (2023)
- 12 A nanocar and rotor in one molecule**
Au-Yeung KH, Sarkar S, Kuhne T, Aiboudi O, Ryndyk DA, Robles R, Lorente N, Lissel F, Joachim C, and Moresco F.
ACS Nano 17, 3128 (2023)
- 13 Optical mirages from spinless beams**
Olmos-Trigo J, Sanz-Fernandez C, Abujetas DR, Garcia-Etxarri A, and Garcia-Martin A.
ACS Photonics 10, 1742 (2023)
- 14 Molecular-induced chirality transfer to plasmonic lattice modes**
Goerlitzer ESA, Zapata-Herrera M, Ponomareva E, Feller D, Garcia-Etxarri A, Karg M, Aizpurua J, and Vogel N.
ACS Photonics 10, 1821 (2023)
- 15 Nonlinear optical response of a plasmonic nanoantenna to circularly polarized light: rotation of multipolar charge density and near-field spin angular momentum inversion**
Quijada M, Babaze A, Aizpurua J, and Borisov AG.
ACS Photonics 10, 3963 (2023)
- 16 Robust rules for optimal colorimetric sensing based on gold nanoparticle aggregation**
Montano-Priede JL, Sanroman-Iglesias M, Zabala N, Grzelczak M, and Aizpurua J.
ACS Sensors 8, 1827 (2023)
- 17 Light-driven self-oscillation of thermoplasmonic nanocolloids**
Mezzasalma SA, Kruse J, Merkens S, Lopez E, Seifert A, Morandotti R, and Grzelczak M.
Advanced Materials 35, 2302987 (2023)
- 18 Dual-phosphorescent heteroleptic silver(I) complex in long-lasting red light-emitting electrochemical cells**
Lipinski S, Cavinato LM, Pickl T, Biffi G, Pothig A, Coto PB, Fernandez-Cestau J, and Costa RD.
Advanced Optical Materials 11, 2203145 (2023)
- 19 Engineering magnetism and superconductivity in van der Waals materials via organic-ion intercalation**
Pereira JM, Tezze D, Ormaza M, Hueso LE, and Gobbi M.
Advanced Physics Research 2, 2200084 (2023)
- 20 On-surface synthesis and characterization of a high-spin aza-[5]-triangulene**
Vilas-Varela M, Romero-Lara F, Vegliante A, Calupitan JP, Martínez A, Meyer L, Uriarte-Amiano U, Friedrich N, Wang D, Schulz F, Koval NE, Sandoval-Salinas ME, Casanova D, Corso M, Artacho E, Peña D, and Pascual JI.
Angewandte Chemie - International Edition 62, e20230788 (2023)

PUBLICATIONS

- 21** **Metamorphosis of a commodity plastic like PVC to efficient catalytic single-chain nanoparticles**
Blazquez-Martín A, Verde-Sesto E, Arbe A, and Pomposo JA.
Angewandte Chemie- International Edition 62, e20231350 (2023)
- 22** **Consecutive single-crystal-to-single-crystal isomerization of novel octamolybdate anions within a microporous hybrid framework with robust water sorption properties**
Ruiz-Bilbao E, Iturrospe A, Reinoso S, Artetxe B, Beobide G, San Felices L, Lezama L, Gutiérrez-Zorrilla JM, Darwish S, and Sensharma D.
Angewandte Chemie-International Edition 62, e2023074 (2023)
- 23** **Triplet odd-frequency superconductivity in hybrid superconductor-ferromagnet structures**
Bergeret FS, and Volkov AF.
Annals of Physics 456, 169232 (2023)
- 24** **Mitigation of efflorescence, drying shrinkage and water demand of calcined clay-based geopolymers with biological waste ashes as activator and hardener**
Oladele OL, Adesanya ED, Arbe A, Iturrospe A, and Ogundiran MB.
Applied Clay Science 243, 107050 (2023)
- 25** **Bipolar thermoelectricity in S/I/NS and S/I/SN superconducting tunnel junctions**
Hijano A, Bergeret FS, Giazotto F, and Braggio A.
Applied Physics Letters 122, 242603 (2023)
- 26** **Switching current distributions in ferromagnetic anomalous Josephson junctions**
Guarcello C, Bergeret FS, and Citro R.
Applied Physics Letters 123, 152602 (2023)
- 27** **Validation of rapid and economic colorimetric nanoparticle assay for SARS-CoV-2 RNA detection in saliva and nasopharyngeal swabs**
Armesto M, Charconnet M, Marimon JM, Regueiro CLF, Jia J, Yan TD, Sorarrain A, Grzelczak M, Sanroman M, Vicente M, Klempa B, Zubiria J, Peng Y, Zhang L, Zhang JH, and Lawrie CH.
Biosensors-Basel 13, 275 (2023)
- 28** **Optical properties of Er³⁺ doped NaLuF₄ transparent glass-ceramics produced by spark plasma sintering**
Sedano M, Balda R, Fernandez J, Duran A, and Pascual MJ.
Ceramics International 49, 41142 (2023)
- 29** **Er/Yb co-doped LiYF₄ transparent oxyfluoride glass-ceramics with up-conversion optical properties**
Truong NMP, Sedano M, Duran A, Balda R, Pascual MJ, and Klement R.
Ceramics International 49, 41201 (2023)
- 30** **An in situ approach to entrap ultra-small iron oxide nanoparticles inside hydrophilic electrospun nanofibers with high arsenic adsorption**
Torasso N, Vergara-Rubio A, Pereira R, Martinez-Sabando J, Baudrit JRV, Cervený S, and Goyanes S.
Chemical Engineering Journal 454, 140168 (2023)

PUBLICATIONS

- 31 Dual crosslinking of low-methoxyl pectin by calcium and europium for the simultaneous removal of pharmaceuticals and divalent heavy metals**
Martínez-Sabando J, Coin F, Raposo JC, Larrañaga A, Melillo JH, and Cervený S.
Chemical Engineering Journal 475, 146162 (2023)
- 32 Unexpected Chain of Redox Events in Co-Based Prussian Blue Analogues**
Morozova PA, Ryazantsev SV, Dembitskiy AD, Morozov AV, Das G, Aquilanti G, Gaboardi M, Plaisier JR, Tsirlin AA, Presniakov IA, Abakumov AM, and Fedotov SS.
Chemistry of Materials 35, 3570 (2023)
- 33 Epitaxial Monolayers of the Magnetic 2D Semiconductor FeBr₂ Grown on Au(111)**
Hadjadj SE, González-Orellana C, Lawrence J, Bikaljevic D, Peña-Díaz M, Gargiani P, Aballe L, Naumann J, Niño MA, Foerster M, Ruiz-Gómez S, Thakur S, Kumberg I, Taylor JM, Hayes J, Torres J, Luo C, Radu F, de Oteyza DG, Kuch W, Pascual JI, Rogero C, and Ilyn M.
Chemistry of Materials 35, 9847 (2023)
- 34 Coupling reversible clustering of DNA-coated gold nanoparticles with chemothermal cycloaddition reaction**
Kruse J, Sanroman-Iglesias M, Marauri A, Rivilla I, and Grzelczak M.
ChemSystemsChem 5, e202200031 (2023)
- 35 Fluid interfaces as models for the study of lipid-based films with biophysical relevance**
Argudo PG, Maestro A, and Guzmán E.
Coatings 13, 1560 (2023)
- 36 Engineering phosphatidylinositol-4,5-bisphosphate model membranes enriched in endocytic cargo: a neutron reflectometry, AFM and QCM-D structural study**
Pereira D, Santamaria A, Pawar N, Carrascosa-Tejedor J, Sardo M, Mafra L, Guzman E, Owen DJ, Zaccai NR, Maestro A, and Marin-Montesinos I.
Colloids and Surfaces B-Biointerfaces 227, 113341 (2023)
- 37 Spin-texture topology in curved circuits driven by spin-orbit interactions**
Hijano A, Rodríguez EJ, Bercieux D, and Frustaglia D.
Communications Physics 6, 186 (2023)
- 38 When matter and information merge into “Quantum”**
Aguado R, Cervera-Lierta A, Correia A, de Franceschi S, Diez Muiño R, Garcia Ripoll JJ, Levi-Yeyati A, Platero G, Roche S, and Sanchez-Portal D.
Communications Physics 6, 266 (2023)
- 39 Tunable Dirac points in a two-dimensional non-symmorphic wallpaper group lattice**
Herrera MAJ, and Bercieux D.
Communications Physics 6, 42 (2023)
- 40 Atomistic simulations, meso-scale analyses and experimental validation of thermal properties in ordinary Portland cement and geopolymers**
Caggiano A, Peralta I, Fachinotti VD, Goracci G, and Dolado JS.
Computers & Structures 285, 107068 (2023)

PUBLICATIONS

- 41 Early-stage analysis of a novel insulation material based on MPCM-doped cementitious foam: Modelling of properties, identification of production process hotspots and exploration of performance trade-offs**
 Zhilyaev D, Fachinotti VD, Zannoni F, Ortega A, Goracci G, Mankel C, Koenders EAB, and Jonkers HM.
 Developments in the Built Environment 16, 100243 (2023)
- 42 A survey of Earth-abundant metal oxides as oxygen evolution electrocatalysts in acidic media (pH < 1)**
 Yu J, Giancola S, Khezri B, Nieto-Castro D, Redondo J, Schiller F, Barja S, Spadaro MC, Arbiol J, García-Pineda FA, Galán-Mascarós JR.
 EES Catalysis 1, 765 (2023)
- 43 B and N substitutional co-doping in 7AGNRs**
 Menchón RE, Delgado-Enales I, Sánchez-Portal D, and Garcia-Lekue A.
 Electronic Structure 5, 045013 (2023)
- 44 Hydrogen spillover in tungsten oxide bronzes as observed by broadband neutron spectroscopy**
 Lalik E, Parker SF, Irvine G, da Silva I, Gutmann MJ, Romanelli G, Druzicki K, Kosydar R, and Krzystyniak M.
 Energies 16, 5496 (2023)
- 45 Tuning the dimensionality of supramolecular materials through the design of peptide-protein co-assemblies**
 Perez-Chirinos L, Sasselli IR, and Cortajarena AL.
 European Biophysics Journal With Biophysics Letters 52, 37 (2023)
- 46 Disentangling the role of electrons and phonons in the photoinduced CO desorption and CO oxidation on (O,CO)-Ru(0001)**
 Tetenoire A, Juaristi JI, and Alducin M.
 Frontiers in Chemistry 11, 1235176 (2023)
- 47 Flavin-conjugated Pt(IV) anticancer agents**
 Sanchez-Camacho J, Infante-Tadeo S, Carrasco AC, Scoditti S, Martinez A, Barroso-Bujans F, Sicilia E, Pizarro AM, and Salassa L.
 Inorganic Chemistry 62, 5644 (2023)
- 48 Structure and luminescent properties of Sm/Dy-doped $\text{Sr}_2\text{MgSi}_2\text{O}_7$ glass-ceramics**
 Fernández-Rodríguez L, Balda R, Fernández J, Durán A, and Pascual MJ.
 International Journal of Applied Glass Science 14, 140 (2023)
- 49 Lattice dynamics of Bi_2Te_3 and vibrational modes in Raman scattering of topological insulators MnBi_2Te_4 center · $n(\text{Bi}_2\text{Te}_3)$**
 Abdullaev NA, Amirasanov IR, Aliev ZS, Jahangirli ZA, Sklyadneva IY, Alizade EG, Aliyeva YN, Otkrov MM, Zverev VN, Mamedov NT, and Chulkov EV.
 JEPT Letters 116, 858 (2023)
- 50 Temperature studies of Raman spectra in MnBi_2Te_4 and MnSb_2Te_4 magnetic topological insulators**
 Maksimov AA, Tartakovskii II, Aliev ZS, Amirasanov IR, Abdullaev NA, Zverev VN, Jahangirli ZA, Sklyadneva IY, Otkrov MM, Mamedov NT, and Chulkov EV.
 JETP Letters 118, 357 (2023)

PUBLICATIONS

- 51 Transport properties of the magnetic topological insulators family $(\text{MnBi}_2\text{Te}_4)(\text{Bi}_2\text{Te}_3)$**
Zverev VN, Abdullayev NA, Aliyev ZS, Amiraslanov IR, Otrokov MM, Mamedov NT, and Chulkov EV.
JETP Letters, Early Access (2023)
- 52 Spark plasma sintering and optical properties of Tm^{3+} and $\text{Tm}^{3+}/\text{Yb}^{3+}$ doped NaLaF_4 transparent glass-ceramics**
Sedano M, Babu S, Balda R, Fernandez J, Duran A, and Pascual MJ.
Journal of Alloys and Compounds 948, 169552 (2023)
- 53 A site-selective fluorescence spectroscopy study of the crystal phases of KY_3F_{10} : leveraging the optical response of Eu^{3+} ions**
Serna-Gallen P, Beltran-Mir H, Cordoncillo E, Balda R, and Fernandez J.
Journal of Alloys and Compounds 953, 170020 (2023)
- 54 Soft ferromagnetic effect in FePc/CdS hybrid diluted magnetic organic/ inorganic quantum dots**
Ibraheem F, El-Bahnasawy H, Mahdy IA, Mahdy MA, Mahmoud EA, Ortega JE, Corso M, Rogero C, and El-Sayed A.
Journal of Alloys and Compounds 968, 171
- 55 Molecular dynamics simulations of the calmodulin-induced alpha-helix in the SK_2 calcium-gated potassium ion channel**
Ramis R, Ballesteros OR, Muguruza-Montero A, M-Alicante S, Nunez E, Villarroel A, Leonardo A, and Bergara A.
Journal of Biological Chemistry 299, 102850 (2023)
- 56 Non-simple flow behavior in a polar van der Waals liquid: Structural relaxation under scrutiny**
Arrese-Igor S, Alegria A, and Colmenero J.
Journal of Chemical Physics 158, 174504 (2023)
- 57 Collective dynamics and self-motions in the van der Waals liquid tetrahydrofuran from meso- to inter-molecular scales disentangled by neutron spectroscopy with polarization analysis**
Arbe A, Nilsen GJ, Devonport M, Farago B, Alvarez F, Gonzalez JAM, and Colmenero J.
Journal of Chemical Physics 158, 184502 (2023)
- 58 Physical aging in molecular glasses beyond the α and β relaxation**
Di Lisio V, Stavropoulou VM, and Cangialosi D.
Journal of Chemical Physics 159, 064505 (2023)
- 59 The Debye's model for the dielectric relaxation of liquid water and the role of cross-dipolar correlations. A MD-simulations study**
Alvarez F, Arbe A, and Colmenero J.
Journal of Chemical Physics 159, 134505 (2023)
- 60 Orbital-free density-functional theory for metal slabs**
Horowitz CM, Proetto CR, and Pitarke JM.
Journal of Chemical Physics 159, 164112 (2023)

PUBLICATIONS

- 61 Unravelling the orientation of the inositol-biphosphate ring and its dependence on phosphatidylinositol 4,5-bisphosphate cluster formation in model membranes**
 Santamaria A, Carrascosa-Tejedor J, Guzmán E, Zaccai NR, and Maestro A.
 Journal of Colloid and Interface Science 629, 785 (2023)
- 62 Investigation on the relationship between lipid composition and structure in model membranes composed of extracted natural phospholipids**
 Santamaria A, Batchu KC, Fragneto G, Laux V, Haertlein M, Darwish TA, Russell RA, Zaccai NR, Guzman E, and Maestro A.
 Journal of Colloid and Interface Science 637, 55 (2023)
- 63 Probing the effect of the capping polyelectrolyte on the internal structure of Layer-by-Layer decorated nanoliposomes**
 Mateos-Maroto A, Rubio JEF, Prevost S, Maestro A, Rubio RG, Ortega F, and Guzman E.
 Journal of Colloid and Interface Science 640, 220 (2023)
- 64 Developing advanced models of biological membranes with hydrogenous and deuterated natural glycerophospholipid mixtures**
 Corucci G, Batchu KC, Luchini A, Santamaria A, Frewein MPK, Laux V, Haertlein M, Yamaryo-Botte Y, Botte CY, Sheridan T, Tully M, Maestro A, Martel A, Porcar L, and Fragneto G.
 Journal of Colloid and Interface Science 645, 870 (2023)
- 65 A numerical study of geopolymer concrete thermal energy storage: Benchmarking TES module design and optimizing thermal performance**
 Rahjoo M, Rojas E, Goracci G, Gaitero JJ, Martauz P, and Dolado JS.
 Journal of Energy Storage-Part B 74, 109389 (2023)
- 66 Marrying plasmonic earth-abundant metals with catalytic metals for visible-light-promoted hydrogen generation on biobased materials**
 Ramírez O, Castillo S, Bonard S, Saldías C, O'Shea JN, Clive CP, Díaz DD, and Leiva A.
 Journal of Environmental Chemistry Engineering 11, 111036 (2023)
- 67 Demonstration of neutrinoless double beta decay searches in gaseous xenon with NEXT**
 Novella P, Sorel M, Usón A, Adams C, Almazán H, Alvarez V, Aparicio B, Aranburu A, Arazi L, Arnquist IJ, Auria-Luna F, Ayet S, Azevedo CDR, Bailey K, Ballester F, del Barrio-Torregrosa M, Bayo A, Benlloch-Rodríguez JM, Borges FIGM, Bounasser S, Byrnes N, Cárcel S, Carrión JV, Cebrián S, Church E, Cid L, Conde CAN, Contreras T, Cossío FP, Dey E, Díaz G, Dickel T, Elorza M, Escada J, Esteve R, Fahs A, Felkai R, Fernandes LMP, Ferrario P, Ferreira AL, Foss FW, Freitas EDC, Freixa Z, Generowicz J, Goldschmidt A, Gómez-Cadenas JJ, González R, Grocott J, Guenette R, Haefner J, Hafidi K, Hauptman J, Henriques CAO, Morata JAH, Herrero-Gómez P, Herrero V, Carrete CH, Ho J, Ho P, Ifergan Y, Jones BJP, Labarga L, Larizgoitia L, Larumbe A, Lebrun P, Lopez F, Gutierrez DL, López-March N, Madigan R, Mano RDP, Marques AP, Martín-Albo J, Martínez-Lema G, Martínez-Vara M, Meziani ZE, Miller RL, Mistry K, Molina-Canteras J, Monrabal F, Monteiro CMB, Mora FJ, Vidal JM, Navarro K, Nuñez A, Nygren DR, Oblak E, Odriozola-Gimeno M, Palacio J, Palmeiro B, Para A, Parmaksiz I, Pelegrin J, Maneiro MP, Querol M, Redwine AB, Renner J, Rivilla I, Rodríguez J, Rogero C, Rogers L, Romeo B, Romo-Luque C, Santos FP, dos Santos JMF, Simón A, Soleti SR, Stanford C, Teixeira JMR, Toledo JF, Torrent J, Veloso JFCA, Vuong TT, Waiton J, and White JT.
 Journal of High Energy Physics 9, 190 (2023)

PUBLICATIONS

68 Reflectance and fluorescence characteristics of PTFE coated with TPB at visible, UV, and VUV as a function of thickness

Haefner J, Fahs A, Ho J, Stanford C, Guenette R, Adams C, Almazan H, Alvarez V, Aparicio B, Aranburu AI, Arazi L, Arnquist IJ, Auria-Luna F, Ayet S, Azevedo CDR, Bailey K, Ballester F, Benlloch-Rodríguez JM, Borges FIGM, Bounasser S, Byrnes N, Carcel S, Carrion JV, Cebrian S, Church E, Conde CAN, Contreras T, Cossio FP, Denisenko AA, Dey E, Diaz G, Dickel T, Escada J, Esteve R, Felkai R, Fernandes LMP, Ferrario P, Ferreira AL, Foss FW, Freitas EDC, Freixa Z, Generowicz J, Goldschmidt A, Gomez-Cadenas JJ, Gonzalez R, Grocott J, Hafidi K, Hauptman J, Henriques CAO, Morata JAH, Herrero-Gomez P, Herrero V, Ho P, Ifergan Y, Jones BJP, Kekic M, Labarga L, Larizgoitia L, Lebrun P, Gutierrez DL, Lopez-March N, Madigan R, Mano RDP, Martin-Albo J, Martinez-Lema G, Martinez-Vara M, Marques AP, Meziani ZE, Miller R, Mistry K, Molina-Canteras J, Monrabal F, Monteiro CMB, Mora FJ, Vidal JM, Navarro K, Novella P, Nunez A, Nygren DR, Oblak E, Odriozola-Gimeno M, Palmeiro B, Para A, Querol M, Redwine AB, Renner J, Rivilla I, Rodriguez J, Rogero C, Rogers L, Romeo B, Romo-Luque C, Santos FP, dos Santos JMF, Simon A, Sorel M, Teixeira JMR, Toledo JF, Torrent J, Uson A, Veloso JFCA, Vuong TT, Waiton J, and White JT. *Journal of Instrumentation* 18, P03016 (2023)

69 A compact dication source for Ba²⁺ tagging and heavy metal ion sensor development

Navarro KE, Baeza-Rubio J, Boyd M, Foss FW, Giri S, Jones BJP, Miller RL, Nygren DR, Samaniego FJ, Stogsdill K, Tiscareno MR, Adams C, Almazán H, Alvarez V, Aparicio B, Aranburu AI, Arazi L, Arnquist IJ, Ayet S, Azevedo CDR, Bailey K, Ballester F, del Barrio-Torregrosa M, Bayo A, Benlloch-Rodríguez JM, Borges FIGM, Bounasser S, Byrnes N, Cárcel S, Carrión JV, Cebrián S, Church E, Cid L, Conde CAN, Contreras T, Cossio FP, Dey E, Díaz G, Dickel T, Elorza M, Escada J, Esteve R, Fahs A, Felkai R, Fernandes LMP, Ferrario P, Ferreira AL, Freitas EDC, Freixa Z, Generowicz J, Goldschmidt A, Gómez-Cadenas JJ, González R, Grocott J, Guenette R, Haefner J, Hafidi K, Hauptman J, Henriques CAO, Morata JAH, Herrero-Gómez P, Herrero V, Carrete CH, Ho J, Ho P, Ifergan Y, Labarga L, Larizgoitia L, Lebrun P, Lopez F, Gutierrez DL, López-March N, Madigan R, Mano RDP, Marques AP, Martín-Albo J, Martínez-Lema G, Martínez-Vara M, Meziani ZE, Mistry K, Monrabal F, Monteiro CMB, Mora FJ, Vidal JM, Novella P, Nuñez A, Oblak E, Odriozola-Gimeno M, Palacio J, Palmeiro B, Para A, Parmaksiz I, Pelegrin J, Maneiro MP, Querol M, Redwine AB, Renner J, Rivilla I, Rodríguez J, Rogero C, Rogers L, Romeo B, Romo-Luque C, Santos FP, dos Santos JMF, Simón A, Soleti SR, Sorel M, Stanford C, Teixeira JMR, Toledo JF, Torrent J, Usón A, Veloso JFCA, Vuong TT, Waiton J, and White. *Journal of Instrumentation* 18, P07044 (2023)

70 NEXT-CRAB-0: a high pressure gaseous xenon time projection chamber with a direct VUV camera based readout

Byrnes NK, Parmaksiz, Adams C, Asaadi J, Baeza-Rubio J, Bailey K, Church E, González-Díaz D, Higley A, Jones BJP, Mistry K, Moya IA, Nygren DR, Oyedele P, Rogers L, Stogsdill K, Almazán H, Alvarez V, Aparicio B, Aranburu AI, Arazi L, Arnquist IJ, Ayet S, Azevedo CDR, Ballester F, del Barrio-Torregrosa M, Bayo A, Benlloch-Rodríguez JM, Borges FIGM, Bounasser S, Cárcel S, Carrión JV, Cebrián S, Cid L, Conde CAN, Contreras T, Cossio FP, Dey E, Díaz G, Dickel T, Elorza M, Escada J, Esteve R, Fahs A, Felkai R, Fernandes LMP, Ferrario P, Ferreira AL, Foss FW, Freitas EDC, Freixa Z, Generowicz J, Goldschmidt A, Gómez-Cadenas JJ, González R, Grocott J, Guenette R, Haefner J, Hafidi K, Hauptman J, Henriques CAO, Morata JAH, Herrero-Gómez P, Herrero V, Carrete CH, Ho J, Ho P, Ifergan Y, Labarga L, Larizgoitia L, Lebrun P, Lopez F, Gutierrez DL, López-March N, Madigan R, Mano RDP, Marques AP, Martín-Albo J, Martínez-Lema G, Martínez-Vara M, Meziani ZE, Miller RL, Monrabal F, Monteiro CMB, Mora FJ, Vidal JM, Navarro KE, Novella P, Nuñez A, Oblak E, Odriozola-Gimeno M, Palacio J, Palmeiro B, Para A, Pelegrin J, Maneiro MP, Querol M, Redwine AB, Renner J, Rivilla I, Rodríguez J, Rogero C, Romeo B, Romo-Luque C, Santos FP, dos Santos JMF, Simón A, Soleti SR, Sorel M, Stanford C, Teixeira JMR, Toledo JF, Torrent J, Usón A, Veloso JFCA, Vuong TT, Waiton J, and White JT. *Journal of Instrumentation* 18, P08006 (2023)

PUBLICATIONS

- 71 MaRCoS, an open-source electronic control system for low-field MRI**
Negnevitsky V, Vives-Gilabert Y, Algarin JM, Craven-Brightman L, Pellicer-Guridi R, O'Reilly T, Stockmann JP, Webb A, Alonso J, and Menkuc B.
Journal of Magnetic Resonance 350, 107424 (2023)
- 72 Ferroelectric control of magnetism of 3d transition metal-adsorbed graphene monolayers**
Wang RQ, Fang YW, and Lei TM.
Journal of Magnetism and Magnetic Materials 565, 170297 (2023)
- 73 Sudden excitations of harmonic normal modes**
Aldazabal I, and Nagy I.
Journal of Mathematical Chemistry 61, 288 (2023)
- 74 Optically active nano-glass-ceramic coatings of Nd³⁺doped-80SiO₂-20LaF₃ prepared by the pre-crystallized nanoparticles sol-gel route**
Cruz ME, Fernandez J, Duran A, Balda R, and Castro Y.
Journal of Non-Crystalline Solids 601, 122050 (2023)
- 75 Characterising the glass transition temperature-structure relationship through a recurrent neural network**
Borredon C, Miccio LA, Cervený S, and Schwartz GA.
Journal of Non-Crystalline Solids: X 18, 100185 (2023)
- 76 The nature of the low-temperature crossover of water in hard confinement**
Beilinson Y, Schiller V, Regentin J, Melillo JH, Greenbaum A, Antropova T, Cervený S, Vogel M, and Feldman Y.
Journal of Physical Chemistry B 127, 5128 (2023)
- 77 Photoinduced CO desorption dominates over oxidation on different O plus CO covered Ru(0001) surfaces**
Tetenoire A, Juaristi JI, and Alducin M.
Journal of Physical Chemistry C 127, 10087 (2023)
- 78 Femtosecond laser-induced desorption of hydrogen molecules from Ru(0001): a systematic study based on machine-learned potentials**
Lindner S, Lončarić I, Vrček L, Alducin M, Juaristi JI, and Saalfrank P.
Journal of Physical Chemistry C 127, 14756 (2023)
- 79 Molecular doping in the organic semiconductor diindenoperylene: insights from many-body perturbation theory**
Mansouri M, Koval P, Sharifzadeh S, and Sanchez-Portal D.
Journal of Physical Chemistry C 127, 16668 (2023)
- 80 Thermal with electronic excitation for the unidirectional rotation of a molecule on a surface**
Au-Yeung KH, Sarkar S, Kuhne T, Aiboudi O, Ryndyk DA, Robles R, Lissel F, Lorente N, Joachim C, and Moresco F.
Journal of Physical Chemistry C 127, 16989 (2023)

PUBLICATIONS

81 Theoretical elastic constants of tobermorite enhanced with reduced graphene oxide through hydroxyl vs epoxy functionalization: a first-principles study

Izadifar M, Dolado JS, Thissen P, Ukrainczyk N, Koenders E, and Ayuela A.
Journal of Physical Chemistry C 127, 18117 (2023)

82 Excitons and their fine structure in lead halide perovskite nanocrystals from atomistic GW/BSE calculations

Biffi G, Cho Y, Krahne R, and Berkelbach TC.
Journal of Physical Chemistry C 127, 1891 (2023)

83 Millifluidic flow reactor for reproducible seed-mediated nanoparticle synthesis

Herrero-Ruiz A, Carolo G, González-Rubio G, Grzelczak M, Niehaus JS, Weller H, and Liz-Marzán LM.
Journal of Physical Chemistry C 127, 19747 (2023)

84 From solution to surface: persistence of the diradical character of a diindenoanthracene derivative on a metallic substrate

Hieulle J, Fernandez CG, Friedrich N, Vegliante A, Sanz S, Sánchez-Portal D, Haley MM, Casado J, Frederiksen T, and Pascual JI.
Journal of Physical Chemistry Letters 14, 11506 (2023)

85 How adsorbed oxygen atoms inhibit hydrogen dissociation on tungsten surfaces

Rodriguez-Fernandez A, Bonnet L, Larregaray P, and Muino RD.
Journal of Physical Chemistry Letters 14, 1246 (2023)

86 Chiral and catalytic effects of site-specific molecular adsorption

Borca B, Michnowicz T, Aguilar-Galindo F, Petuya R, Pristl M, Schendel V, Pentegov I, Kraft U, Klauk H, Wahl P, Arnau A, and Schlickum U.
Journal of Physical Chemistry Letters 14, 2072 (2023)

87 Room-temperature C-C sigma-bond activation of biphenylene derivatives on Cu(111)

Calupitan JP, Wang T, Paz AP, Alvarez B, Berdonces-Layunta A, Angulo-Portugal P, Castrillo-Bodero R, Schiller F, Pena D, Corso M, Perez D, and de Oteyza DG.
Journal of Physical Chemistry Letters 14, 947 (2023)

88 Adsorption of silanediol-like molecules on TiO₂ nano-clusters: A density-functional-theoretic study

Aguilera-Granja F, Aguilera-del-Toro RH, Vogel EE, and Escrig J.
Journal of Physics and Chemistry of Solids 183, 111642 (2023)

89 Association of oppositely charged polyelectrolyte and surfactant in solution: equilibrium and nonequilibrium features

Guzman E, Maestro A, Ortega F, and Rubio RG.
Journal of Physics-Condensed Matter 35, 323001 (2023)

90 Understanding the effect of MPEG-PCE's microstructure on the adsorption and hydration of OPC

Emaldi I, Erkizia E, Leiza JR, and Dolado JS.
Journal of the American Chemical Society 106, 2567 (2023)

PUBLICATIONS

- 91** **Tuning the diradical character of pentacene derivatives via non-benzenoid coupling motifs**
Wang T, Angulo-Portugal P, Berdonces-Layunta A, Jancarik A, Gourdon A, Holec J, Kumar M. Soler D, Jelinek P, Casanova D, Corso M, Oteyza DGD, and Calupitan JP.
Journal of the American Chemical Society 145, 10333 (2023)
- 92** **Chemical and interfacial design in the visible-light-absorbing ferroelectric thin films**
Cheng XR, Xi GQ, Fang YW, Ding JQ, Tian JJ, and Zhang LX.
Journal of the European Ceramic Society 43, 3275 (2023)
- 93** **Mach-Zehnder-like interferometry with graphene nanoribbon networks**
Sanz S, Papior N, Giedke G, Sanchez-Portal D, Brandbyge M, and Frederiksen T.
Journals of Physics-Condensed Matter 35, 374001 (2023)
- 94** **Effects of charge density on spread hyperbranched polyelectrolyte/surfactant films at the air/water interface**
Carrascosa-Tejedor J, Tummino A, Fehér B, Kardos A, Efstratiou M, Skoda MWA, Gutfreund P, Maestro A, Lawrence MJ, Campbell RA, and Varga I.
Langmuir 39, 14869 (2023)
- 95** **The effect of chain topology on the crystallization and polymorphism of PVDF: linear versus star molecules**
Algarni F, Zapsas G, Maria N, Maiz J, Muller AJ, and Hadjichristidis N.
Macromolecular Chemistry and Physics 224, 2200268 (2023)
- 96** **Rationalizing the effect of the MAA/PEGMA ratio of comb-shape copolymers synthesized by aqueous free-radical copolymerization in the hydration kinetics of ordinary portland cements**
Beldarrain S, Barquero A, Goracci G, Dolado JS, and Leiza JR.
Macromolecular Materials and Engineering, 230032 (2023)
- 97** **Microscopic versus macroscopic glass transitions and relevant length scales in mixtures of industrial interest**
Arbe A, Colmenero J, Shafqat N, Alegria A, Malicki N, Dronet S, Natali F, Mangin-Thro L, and Porcar L.
Macromolecules 56, 2149 (2023)
- 98** **Amphiphilic polymer conetworks studied by SANS: effect of the type of solubilize and molecular architecture on the swollen gel structure**
de Molina PM, Kafouris D, Patrickios CS, Noirez L, and Gradzielski M.
Macromolecules 56, 8323 (2023)
- 99** **Structure of single-chain nanoparticles under crowding conditions: a random phase approximation approach**
Robles-Hernández B, González-Burgos M, de Molina PM, Asenjo-Sanz I, Radulescu A, Pomposo JA, Arbe A, and Colmenero J.
Macromolecules 56, 8971 (2023)
- 100** **Understanding continuous wave laser-induced chemical reactions at micro- and nano-diamond-glass interface under infrared excitation**
Zemojtel P, Olejniczak A, Tomala R, Cichy B, Radosinski L, Maia AFD, Bezkravnyi O, and Strek W.
Material Research Express 10, 095601 (2023)

PUBLICATIONS

- 101 A review of pectin-based material for applications in water treatment**
Martinez-Sabando J, Coin F, Melillo JH, Goyanes S, and Cervený S.
Materials 6, 2207 (2023)
- 102 Anion-induced robust ferroelectricity in sulfurized pseudo-rhombohedral epitaxial BiFeO₃ thin films via polarization rotation**
Xi GQ, Pan Z, Fang YW, Tu J, Li HR, Yang QQ, Liu C, Luo HJ, Ding JQ, Xu S, Deng SQ, Wang QX, Zheng DX, Long YW, Jin KJ, Zhang XX, Tian JJ, and Zhang LX.
Materials Horizons 10, 4389 (2023)
- 103 Etch and growth rates of GaN for surface orientations in the crystallographic zone: Step flow and terrace erosion/filling via the Continuous Cellular Automaton**
Guo XY, Gosálvez MA, Xing Y, and Chen Y.
Materials Science in Semiconductor Processing 153, 107173 (2023)
- 104 Designing ternary superconducting hydrides with A15-type structure at moderate pressures**
Wei XD, Hao XK, Bergara A, Zurek E, Liang XW, Wang LY, Song XX, Li PF, Wang L, Gao GY, and Tian YJ.
Materials Today Physics 34, 101086 (2023)
- 105 Pressure-induced evolution of stoichiometries and electronic structures of host-guest Na-B compounds**
Guo ZX, Li X, Bergara A, Ding SC, Zhang XH, and Yang GC.
Matter and Radiation at Extremes 8, 068401
- 106 Adsorption of methylene blue and tetracycline by zeolites immobilized on a PBAT electrospun membrane**
Picon D, Vergara-Rubio A, Estevez-Areco S, Cervený S, and Goyanes S.
Molecules 28, 81 (2023)
- 107 Quantum plasmonics in sub-atom-thick optical slots**
Baumberg JJ, Esteban R, Hu S, Muniain U, Silkin IV, Aizpurua J, and Silkin VM.
Nano Letters 23, 10696 (2023)
- 108 Thioetherification of Br-mercaptobiphenyl molecules on Au(111)**
Barragan A, Robles R, Vitali L, and Lorente N.
Nano Letters 23, 1350 (2023)
- 109 Anharmonicity reveals the tunability of the charge density wave orders in monolayer VSe₂**
Fumega AO, Diego J, Pardo V, Blanco-Canosa S, and Errea I.
Nano Letters 23, 1794 (2023)
- 110 Gate-tunable spin Hall effect in an all-light-element heterostructure: Graphene with copper oxide**
Yang HZ, Ormaza M, Chi ZD, Dolan E, Ingla-Aynes J, Safeer CK, Herling F, Ontoso N, Gobbi M, Martin-Garcia B, Schiller F, Hueso LE, and Casanova F.
Nano Letters 23, 4406 (2023)
- 111 Emergence of π -magnetism in fused aza-triangulenes: symmetry and charge transfer effects**
Calupitan JP, Berdonces-Layunta A, Aguilar-Galindo F, Vilas-Varela M, Peña D, Casanova D, Corso M, de Oteyza DG, and Wang T.
Nano Letters 23, 9832 (2023)

PUBLICATIONS

- 112** **Toward long-term-dispersible, metal-free single-chain nanoparticles**
Blazquez-Martin A, Ruiz-Bardillo A, Verde-Sesto E, Iturrospe A, Arbe A, and Pomposo JA.
Nanomaterials 13, 1394 (2023)
- 113** **Acoustic plasmons in nickel and its modification upon hydrogen uptake**
Koroteev YM, Silkin IV, Chernov IP, Chulkov EV, and Silkin VM.
Nanomaterials 13, 141 (2023)
- 114** **Dimerization effects and negative strain energy in silicon monosulfide nanotubes**
Alonso-Lanza T, Aguilera-Granja F, and Ayuela A.
Nanomaterials 13, 3033 (2023)
- 115** **Superlattices of gadolinium and bismuth based thallium dichalcogenides as potential magnetic topological insulators**
Vyazovskaya AY, Petrov EK, Koroteev YM, Bosnar M, Silkin IV, Chulkov EV, and Otrokov MM.
Nanomaterials 13, 38 (2023)
- 116** **Effects of the spatial extension of the edge channels on the Interference Pattern of a Helical Josephson Junction**
Vigliotti L, Calzona A, Ziani NT, Bergeret FS, Sassetti M, and Trauzettel B.
Nanomaterials 13, 569 (2023)
- 117** **Novel sol-gel route to prepare Eu^{3+} -doped 80SiO_2 - 20NaGdF_4 oxyfluoride glass-ceramic for photonic device applications**
Cruz ME, Tran TNL, Chiasera A, Duran A, Fernandez J, Balda R, and Castro Y.
Nanomaterials 13, 940 (2023)
- 118** **Dispersive surface-response formalism to address nonlocality in extreme plasmonic field confinement**
Babaze A, Neuman T, Esteban R, Aizpurua J, and Borisov AG.
Nanophotonics 12, 3277 (2023)
- 119** **Control of the structure and morphology of polypeptide/surfactant spread films by exploiting specific interactions**
Carrascosa-Tejedo J, Minarro LM, Efstratiou M, Varga I, Skoda MWA, Gutfreund P, Maestro A, Lawrence MJ, and Campbell RA.
Nanoscale 15, 11141 (2023)
- 120** **A ferromagnetic Eu-Pt surface compound grown below hexagonal boron nitride**
Bakhit AMI, Ali K, Makarova AA, Pis I, Bondino F, Sant R, Dash SP, Castrillo-Bodero R, Hasegawa Y, Ortega JE, Fernandez L, and Schiller F.
Nanoscale 15, 11517 (2023)
- 121** **Electronic band structure of 1D pi-d hybridized narrow-gap metal-organic polymers**
Frezza F, Schiller F, Cahlik A, Ortega JE, Barth JV, Arnau A, Blanco-Rey M, Jelinek P, Corso M, and Piquero-Zulaica I.
Nanoscale 15, 2285 (2023)

PUBLICATIONS

- 122** **Tuning the carrier injection barrier of hybrid metal-organic interfaces on rare earth-gold surface compounds**
Castrillo-Bodero R, Blanco-Rey M, Ali K, Ortega JE, Schiller F, and Fernandez L.
Nanoscale 15, 4090 (2023)
- 123** **Self-assembled three-dimensional hydrogels based on graphene derivatives and cerium oxide nanoparticles: scaffolds for co-culture of oligodendrocytes and neurons derived from neural stem cells**
Polo Y, Luzuriaga J, de Langerica SG, Pardo-Rodriguez B, Martinez-Tong DE, Tapeinos C, Manero-Roig I, Marin E, Munoz-Ugartemendia J, Ciofani G, Ibarretxe G, Unda F, Sarasua JR, Pineda JR, and Larranaga A.
Nanoscale 15, 4488 (2023)
- 124** **Magnetic order and magnetic anisotropy in two-dimensional ilmenenes**
Aguilera-del-Toro RH, Arruabarrena M, Leonardo A, and Ayuela A.
Nanoscale Advances 5, 2813 (2023)
- 125** **Insight into the electronic structure of the centrosymmetric skyrmion magnet GdRu_2Si_2**
Eremeev SV, Glazkova D, Poelchen G, Kraiker A, Ali K, Tarasov AV, Schulz S, Kliemt K, Chulkov EV, Stolyarov VS, Ernst A, Krellner C, Usachov DY, and Vyalikh DV.
Nanoscale Advances 5, 6678 (2023)
- 126** **Quantum structural fluxion in superconducting lanthanum polyhydride**
Wang H, Salzbrenner PT, Errea I, Peng F, Lu ZH, Liu HY, Zhu L, Pickard CJ, and Yao YS.
Nature Communications 14, 1674 (2023)
- 127** **Giant optomechanical spring effect in plasmonic nano- and picocavities probed by surface-enhanced Raman scattering**
Jakob LA, Deacon WM, Zhang Y, de Nijs B, Pavlenko E, Hu S, Carnegie C, Neuman T, Esteban R, Aizpurua J, and Baumberg JJ.
Nature Communications 14, 3291 (2023)
- 128** **Excitonic insulator to superconductor phase transition in ultra-compressed helium**
Liu C, Errea I, Ding C, Pickard C, Conway LJ, Monserrat B, Fang YW, Lu Q, Sun J, and Boronat J.
Nature Communications 14, 4458 (2023)
- 129** **Size-dependent vitrification in metallic glasses**
Di Lisio V, Gallino I, Riegler SS, Frey M, Neuber N, Kumar G, Schroers J, Busch R, and Cangialosi D.
Nature Communications 14, 4698 (2023)
- 130** **Long-lived spin waves in a metallic antiferromagnet**
Poelchen G, Hellwig J, Peters M, Usachov DY, Kliemt K, Laubschat C, Echenique PM, Chulkov EV, Krellner C, Parkin SSP, Vyalikh DV, Ernst A, and Kummer K.
Nature Communications 14, 5422 (2023)
- 131** **Photoluminescence upconversion in monolayer WSe_2 activated by plasmonic cavities through resonant excitation of dark excitons**
Mueller NS, Arul R, Kang G, Saunders AP, Johnson AC, Sánchez-Iglesias A, Hu S, Jakob LA, Bar-David J, de Nijs B, Liz-Marzán LM, Liu F, and Baumberg JJ.
Nature Communications 14, 5726 (2023)

PUBLICATIONS

- 132 Detecting the spin-polarization of edge states in graphene nanoribbons**
Brede J, Merino-Díez N, Berdonces-Layunta A, Sanz S, Domínguez-Celorrio A, Lobo-Checa J, Vilas-Varela M, Peña D, Frederiksen T, Pascual JI, de Oteyza DG, and Serrate D.
Nature Communications 14, 6677 (2023)
- 133 Evidence for ground state coherence in a two-dimensional Kondo lattice**
Wan W, Harsh R, Meninno A, Dreher P, Sajan S, Guo H, Errea I, de Juan F, and Ugeda MM.
Nature Communications 14, 7005 (2023)
- 134 Local control of superconductivity in a NbSe₂/CrSBr van der Waals heterostructure**
Jo J, Peisen Y, Yang H, Manas-Valero S, Baldovi JJ, Lu Y, Coronado E, Casanova F, Bergeret FS, Gobbi M, and Hueso LE.
Nature Communications 14, 7256 (2023)
- 135 Probing optical anapoles with fast electron beams**
Maciel-Escudero C, Yankovich AB, Munkhbat B, Baranov DG, Hillenbrand R, Olsson E, Aizpurua J, and Shegai TO.
Nature Communications 14, 8478 (2023)
- 136 Record high room temperature resistance switching in ferroelectric-gated Mott transistors unlocked by interfacial charge engineering**
Hao Y, Chen X, Zhang L, Han MG, Wang W, Fang YW, Chen H, Zhu Y, and Hong X.
Nature Communications, 14, 8247 (2023)
- 137 Real-space observation of ultraconfined in-plane anisotropic acoustic terahertz plasmon polaritons**
Chen S, Leng PL, Konecna A, Modin E, Gutierrez-Amigo M, Vicentini E, Martin-Garcia B, Barra-Burillo M, Niehues I, Escudero CM, Xie XY, Hueso LE, Artacho E, Aizpurua J, Errea I, Vergniory MG, Chuvilin A, Xiu FX, and Hillenbrand R.
Nature Materials 22, 860 (2023)
- 138 A New Frontier: high-pressure Neutron Science on TOSCA**
Armstrong J, Wang X, and Fernandez-Alonso F.
Neutron News 34, 4 (2023)
- 139 Benchmarking the performance of a low-cost magnetic resonance control system at multiple sites in the open MaRCoS community**
Guallart-Naval T, O'Reilly T, Algarin JM, Pellicer-Guridi R, Vives-Gilabert Y, Craven-Brightman L, Negnevitsky V, Menkuc B, Galve F, Stockmann JP, Webb A, and Alonso J.
NMR in Biomedicine 36, e4825 (2023)
- 140 Open-source magnetic resonance imaging: Improving access, science, and education through global collaboration**
Winter L, Periquito J, Kolbitsch C, Pellicer-Guridi R, Nunes RG, Haeuer M, Broche L, and O'Reilly T.
NMR in Biomedicine, Early Access (2023)
- 141 High Chern number van der Waals magnetic topological multilayers MnBi₂Te₄/hBN**
Bosnar M, Vyazovskaya AY, Petrov EK, Chulkov EV, and Otrokov MM.
NPJ 2D Materials and Applications 7, 33 (2023)

PUBLICATIONS

- 142 Superconducting dome by tuning through a van Hove singularity in a two-dimensional metal**
Wan W, Harsh R, Dreher P, de Juan F, and Ugeda MM.
NPJ 2D Materials and Applications 7, 41 (2023)
- 143 Nonlinear optical properties of 3,3'-biindole 2,2' (1H,1'H)-dione derivatives**
Zarif FA, Esmaeili AA, Zeraatkar Z, Behrouz M, Dehghani Z, Miccio LA, and Sharifi S.
Optical and Quantum Electronics 55, 768 (2023)
- 144 Role of the thermal treatment on the microstructure of YAGG nanopowders prepared by urea glass route**
Armetta F, Gaboardi M, Plaisier J, and Saladino ML.
Optical Materials 140, 113896 (2023)
- 145 High colour rendering index and warm emission of conventional white-LED capped with metal-phthalocyanine/CdSe nanocomposites**
Elkalashy O, Ibraheem F, Said SA, Mohamed SA, El-Hamalawy A, Al-Kamel AN, Khalil MS, and El-Sayed A.
Optical Materials 146, 114495 (2023)
- 146 Fano asymmetry in zero-detuned exciton-plasmon systems**
Nodar A, Neuman T, Zhang Y, Aizpurua J, and Esteban R.
Optics Express 31, 10297 (2023)
- 147 Suppressed-scattering spectral windows for radiative cooling applications**
Perez-Escudero JM, Torres-Garcia AE, Lezaun C, Caggiano A, Peralta I, Dolado JS, Beruete M, and Liberal I.
Optics Express 31, 6314 (2023)
- 148 Spectro-temporal behavior of dye-based solid-state random lasers under a picosecond pumping regime: Part III**
Iparraguirre I, Garcia-Revilla S, Azkargorta J, Fernandez J, and Balda R.
Optics Express 31, 7159 (2023)
- 149 First-principles design of ferromagnetic monolayer MnO₂ at the complex interface**
Wang RQ, Lei TM, and Fang YW.
Physica Scripta 98, 065960 (2023)
- 150 Emergent superconductivity in TaO₃ at high pressures**
Li WJ, Li X, Zhang XH, Yu H, Han FJJ, Bergara A, Lin JY, Wu JH, and Yang GC.
Physical Chemistry Chemical Physics 25, 23502 (2023)
- 151 A Janus CrSSe monolayer with interesting ferromagnetism**
Han FJJ, Yan X, Bergara A, Li WJ, Yu H, and Yang GC.
Physical Chemistry Chemical Physics 25, 29672 (2023)
- 152 Simulating high-pressure surface reactions with molecular beams**
Taleb AA, Schiller F, Vyalikh DV, Pérez JM, Auras SV, Farias D, and Ortega JE.
Physical Chemistry Chemical Physics 26, 1770 (2023)

PUBLICATIONS

- 153 Influence of direct dipole-dipole interactions on the optical response of two-dimensional materials in strongly inhomogeneous infrared cavity fields**
Ribeiro S, Aizpurua J, and Esteban R.
Physical Review A 108, 043718 (2023)
- 154 Microwave-assisted thermoelectricity in S-I-S' tunnel junctions**
Hijano A, Bergeret FS, Giazotto F, and Braggio A.
Physical Review Applied 19, 044024 (2023)
- 155 Prediction of monolayer FeP_4 with intrinsic half-metal ferrimagnetism above room temperature**
Han FJJ, Yan X, Li F, Yu H, Li WJ, Zhong X, Bergara A, and Yang GC.
Physical Review B 107, 024414 (2023)
- 156 Ab initio study of metastable occupation of tetrahedral sites in palladium hydrides and its impact on superconductivity**
Meninno A, and Errea I.
Physical Review B 107, 024504 (2023)
- 157 Secondary electron emission in the scattering of fast probes by metallic interfaces**
Rivacoba A.
Physical Review B 107, 0345401 (2023)
- 158 Optomechanical effects in nanocavity-enhanced resonant Raman scattering of a single molecule**
Shen XM, Zhang Y, Zhang SP, Zhang Y, Meng QS, Zheng GC, Lv SY, Wang LX, Boto RA, Shan CX, and Aizpurua J.
Physical Review B 107, 075435 (2023)
- 159 Anisotropic differential conductance of a mixed-parity superconductor/ferromagnet structure**
Kokkeler T, Hijano A, and Bergeret FS.
Physical Review B 107, 104506 (2023)
- 160 Topological phonon analysis of the two-dimensional buckled honeycomb lattice: An application to real materials**
Gutierrez-Amigo M, Vergniory MG, Errea I, and Manes JL.
Physical Review B 107, 144307 (2023)
- 161 Microscopic theory of spin relaxation of a single Fe adatom coupled to substrate vibrations**
Garai-Marin H, Dias MD, Lounis S, Ibanez-Azpiroz J, and Eiguren A.
Physical Review B 107, 144417 (2023)
- 162 Paradoxical effects for a one-dimensional periodic potential embedded in a two-dimensional system**
Kolpatzeck K, Brendel L, Moeller R, Robles R, and Lorente N.
Physical Review B 107, 155418 (2023)
- 163 Introduction of localized spin-state transitions in the optical absorption spectrum of Cr-doped GaN**
Mansouri M, Lewis DK, and Sharifzadeh S.
Physical Review B 107, 184103 (2023)

PUBLICATIONS

- 164** **Emergence of large spin-charge interconversion at an oxidized Cu/W interface**
Groen I, Pham V, Ilic S, Chuvilin A, Choi WY, Sagasta E, Vaz DC, Arango IC, Ontoso N, Bergeret FS, Hueso LE, Tokatly IV, and Casanova F.
Physical Review B 107, 184438 (2023)
- 165** **Towards a universal exchange enhancement factor in density functional theory**
Horowitz CM, Proetto CR, and Pitarke JM.
Physical Review B 107, 195120 (2023)
- 166** **Including many-body effects into the Wannier-interpolated quadratic photoresponse tensor**
Garcia-Goiricelaya P, Krishna J, and Ibanez-Azpiroz J.
Physical Review B 107, 205101 (2023)
- 167** **Ab initio study of the nonlinear optical properties and dc photocurrent of the Weyl semimetal TaIrTe₄**
Puente-Uriona AR, Tsirkin SS, Souza I, and Ibanez-Azpiroz J.
Physical Review B 107, 205204 (2023)
- 168** **Robust spin polarization of Yu-Shiba-Rusinov states in superconductor/ferromagnetic insulator heterostructures**
Skurativska A, Ortuzar J, Bercieux D, Bergeret FS, and Cazalilla MA.
Physical Review B 107, 224597 (2023)
- 169** **Many-body nonequilibrium effects in all-electric electron spin resonance**
Reina-Galvez J, Wolf C, and Lorente N.
Physical Review B 107, 235404 (2023)
- 170** **Superconductivity in Li₈Au electride**
Zhang XH, Yao YS, Ding SC, Bergara A, Li F, Liu Y, Zhou XF, and Yang GC.
Physical Review B 107, L100501 (2023)
- 171** **Anomalous transient blueshift in the internal stretch mode of CO/Pd(111)**
Bombin R, Muzas AS, Novko D, Juaristi JI, and Alducin M.
Physical Review B 107, L121404 (2023)
- 172** **Theory of a single magnetic impurity on a thin metal film in proximity to a superconductor**
Ortuzar J, Pascual JI, Bergeret S, and Cazalilla MA.
Physical Review B 108, 024511 (2023)
- 173** **Vibrational dynamics of CO on Pd(111) in and out of thermal equilibrium**
Bombin R, Muzas AS, Novko D, Juaristi JI, and Alducin M.
Physical Review B 108, 045409 (2023)
- 174** **Ab initio study of the structural, vibrational, and optical properties of potential parent structures of nitrogen-doped lutetium hydride**
Dangić Đ, Garcia-Goiricelaya P, Fang YW, Ibañez-Azpiroz J, and Errea I.
Physical Review B 108, 064517 (2023)
- 175** **Proximity effect of time-reversal symmetry broken noncentrosymmetric superconductors**
Kokkeler T, Golubov A, Bergeret S, and Tanaka Y.
Physical Review B 108, 094503 (2023)

PUBLICATIONS

- 176 Interstitial anionic electrons favoring superconductivity in Li-As electrides**
Zhao YP, Bergara A, Zhang XH, Li F, Liu Y, and Yang GC.
Physical Review B 108, 104505 (2023)
- 177 Dynamical Hall responses of disordered superconductors**
Hijano A, Vosoughi-nia S, Bergeret FS, Virtanen P, and Heikkilä TT.
Physical Review B 108, 104506 (2023)
- 178 Construction of a semilocal exchange density functional from a three-dimensional electron gas collapsing to two dimensions**
Horowitz CM, Proetto CR, and Pitarke JM.
Physical Review B 108, 115119 (2023)
- 179 Shift photoconductivity in the Haldane model**
Sivianes J, and Ibañez-Azpiroz J.
Physical Review B 108, 155419 (2023)
- 180 Understanding the large shift photocurrent of WS₂ nanotubes: a comparative analysis with monolayers**
Krishna J, Garcia-Goiricelaya P, de Juan F, and Ibañez-Azpiroz J.
Physical Review B 108, 165418 (2023)
- 181 Spectral properties of disordered Ising superconductors with singlet and triplet pairing in in-plane magnetic fields**
Ilic S, Meyer JS, and Houzet M.
Physical Review B 108, 214510 (2023)
- 182 Magnon currents excited by the spin Seebeck effect in ferromagnetic EuS thin films**
Aguilar-Pujol MX, Catalano S, Gonzalez-Orellana C, Skowronski W, Gomez-Perez JM, Ilyn M, Rogero C, Gobbi M, Hueso LE, and Casanova F.
Physical Review B 108, 224420 (2023)
- 183 Reducing the frequency of the Higgs mode in a helical superconductor coupled to an LC circuit**
Lu Y, Ilic S, Ojajärvi R, Heikkilä TT, and Bergeret FS.
Physical Review B 108, 224517 (2023)
- 184 Wigner-Seitz truncated time-dependent density functional theory approach for the calculation of exciton binding energies in solids**
Arruabarrena M, Leonardo A, and Ayuela A.
Physical Review B 108, 235210 (2023)
- 185 Spectroscopic signature of spin triplet odd-valley superconductivity in two-dimensional materials**
Kokkeler TH, Huang CL, Bergeret FS, and Tokatly IV.
Physical Review B 108, L180504 (2023)
- 186 Ferromagnetic ordering of magnetic impurities mediated by supercurrents in the presence of spin-orbit coupling**
Lu Y, Tokatly I, and Bergeret SF.
Physical Review B 108, L180506 (2023)

PUBLICATIONS

- 187 Cooper pair excitation mediated by a molecular quantum spin on a superconducting proximitized gold film**
Trivini S, Ortuzar J, Vaxevani K, Li JC, Bergeret FS, Cazalilla MA, and Pascual JI.
Physical Review Letters 130, 136004 (2023)
- 188 Ubiquitous superconducting diode effect in superconductor thin films**
Hou YS, Nichele F, Chi H, Lodesani A, Wu YY, Ritter MF, Haxell DZ, Davydova M, Ilic S, Glezakou-Elbert O, Varambally A, Bergeret S, Kamra A, Fu L, Lee PA, and Moodera JS.
Physical Review Letters 131, 027001 (2023)
- 189 Energy-overlap of the Dirac surface state with bulk bands in SnBi_2Te_4**
Eremeev SV, De Luca O, Sheverdyeva PM, Ferrari L, Matetskiy AV, Di Santo G, Petaccia L, Crovara C, Caruso T, Papagno M, Agostino RG, Aliev ZS, Moras P, Carbone C, Chulkov EV, and Pacile D.
Physical Review Materials 7, 014203 (2023)
- 190 Quantum tunneling rotor as a sensitive atomistic probe of guests in a metal-organic framework**
Titov K, Ryder MR, Lemaire A, Zeng ZX, Chaudhari AK, Taylor J, Mahdi EM, Rogge SMJ, Mukhopadhyay S, Rudic S, Van Speybroeck V, and Fernandez-Alonso F.
Physical Review Materials 7, 073402 (2023)
- 191 Floating of the topological surface state on top of a thick lead layer: The case of the $\text{Pb}/\text{Bi}_2\text{Se}_3$ interface**
De Luca O, Shvets IA, Eremeev SV, Aliev ZS, Kopciuszynski M, Barinov A, Ronci F, Colonna S, Chulkov EV, Agostino RG, Papagno M, and Flammini R.
Physical Review Materials 7, 124203 (2023)
- 192 Resonant helicity mixing of electromagnetic waves propagating through matter**
Lasa-Alonso J, Olmos-Trigo J, Devescovi C, Hernandez P, Garcia-Etxarri A, and Molina-Terriza G.
Physical Review Research 5, 023116 (2023)
- 193 Probing the electromagnetic response of dielectric antennas by vortex electron beams**
Konecna A, Schmidt MK, Hillenbrand R, and Aizpurua J.
Physical Review Research 5, 023192 (2023)
- 194 Bipolar single-molecule electroluminescence and electrofluorochromism**
Hung TC, Robles R, Kiraly B, Strik JH, Rutten BA, Khajetoorians AA, Lorente N, and Wegner D.
Physical Review Research 5, 033027 (2023)
- 195 Nonlinear electronic stopping of negatively charged particles in liquid water**
Koval NE, Da Pieve F, Gu B, Munoz-Santiburcio D, Kohanoff J, and Artacho E.
Physical Review Research 5, 033063 (2023)
- 196 Identifying unbound strong bunching and the breakdown of the rotating wave approximation in the quantum Rabi model**
Nodar A, Esteban R, Muniain U, Steel MJ, Aizpurua J, and Schmidt MK.
Physical Review Research 5, 043213 (2023)
- 197 Self-propelling colloids with finite state dynamics**
van Kesteren S, Alvarez L, Arrese-Igor S, Alegria A, and Isa L.
PNAS 120, e2213481120 (2023)

PUBLICATIONS

- 198 Segmental dynamics of poly(tetrahydrofuran) cross-linked by click-chemistry: Single-chain nanoparticles vs cross-linked networks**
Sharifi S, Asenjo-Sanz I, Verde-Sesto E, Maiz J, Pomposo JA, and Alegría A.
Polymer 287, 126422 (2023)
- 199 Extended detailed balance modeling toward solar cells with cement-based radiative coolers**
Cagnoni M, Testa P, Dolado JS, and Cappelluti F.
Progress in Photovoltaics, Early Access (2023)
- 200 Ferroelectricity in layered bismuth oxide down to 1 nanometer**
Yang QQ, Hu JC, Fang YW, Jia YY, Yang R, Deng SQ, Lu Y, Dieguez O, Fan LL, Zheng DX, Zhang XX, Dong YQ, Luo ZL, Wang Z, Wang HH, Sui ML, Xing XR, Chen J, Tian JJ, and Zhang LX.
Science 379, 1218 (2023)
- 201 An atomic-scale multi-qubit platform**
Wang Y, Chen Y, Bui HT, Wolf C, Haze M, Mier, C, Kim, J, Choi, DJ, Lutz CP, Bae Y, Phark SH, and Heinrich AJ.
Science 382, 87 (2023)
- 202 CLIP-Seq analysis enables the design of protective ribosomal RNA bait oligonucleotides against C9ORF72 ALS/FTD poly-GR pathophysiology**
Ortega JA, Sasselli IR, Boccitto M, Fleming A, Fortuna TR, Li Y, Sato K, Clemons TD, McKenna ED, Nguyen TP, Anderson EN, Asin J, Ichida JK, Pandey UB, Wolin SL, Stupp SI, and Kiskinis E.
Science Advances 9, eadf7997 (2023)
- 203 Localization versus delocalization of d-states within the Ni_2MnGa (Correction)**
Janovec J, Zeleny M, Heczko O, and Ayuela A.
Scientific Reports (Correction) 12, 20577 (2023)
- 204 Multipole theory of optical spatial dispersion in crystals**
Ocana OP, and Souza I.
Scipost Physics 14, 118 (2023)
- 205 Theoretical study of structural, electronic and magnetic properties of Co clusters embedded in an Ag matrix**
Aguilera-Granja F, Torres MB, and Aguilera-del-Toro RH.
Solid State Communications 372, 115301 (2023)
- 206 Sulfites detection by surface-enhanced Raman spectroscopy: A feasibility study**
Villar A, Merino S, Boto RA, Aizpurua J, Garcia A, Azkune M, and Zubia J.
Spectrochimica Acta Part-A Molecular and Biomolecular Spectroscopy 300, 122899 (2023)
- 207 Superconductor-ferromagnet hybrids for non-reciprocal electronics and detectors**
Geng Z, Hijano A, Ilic S, Ilyn M, Maasilta I, Monfardini A, Spies M, Strambini E, Virtanen P, Calvo M, González-Orellána C, Helenius A P, Khorshidian S, Levartoski de Araujo C I, Levy-Bertrand F, Rogero C, Giazotto F, Bergeret FS, and Heikkilä T T.
Superconductor Science and Technology 36, 123001 (2023)
- 208 A study of step defects on $\text{NiAl}(110)$ using a curved single crystal surface**
Pineiros-Bastidas JM, Auras SV, and Juurlink LBF.
Surface Science 732, 122270 (2023)

PUBLICATIONS

- 209** **Fast scanning calorimetry on volatile carbon-based materials**
Di Lizio V, Braunewell, B, Macia-Castello C, Simoni M, Senesi R, Fernandez-Alonso F, and Cangialosi D.
Thermochimica Acta 719, 179414 (2023)
- 210** **Quantification of reagent mixing in liquid flow cells for Liquid Phase-TEM**
Merkens S, De Salvo G, Kruse J, Modin E, Tollan C, Grzelczak M, and Chuvilin A.
Ultramicroscopy 245, 113654 (2023)
- 211** **On energetics of allotrope transformations in transition-metal diborides via plane-by-plane shearing**
Leiner T, Koutna N, Janovec J, Zeleny M, Mayrhofer PH, and Holec D.
Vacuum 215, 112329 (2023)

PATENTS APPLIED FOR

Flow cells for liquid-phase transmission electron microscopy and methods

EP23382771.6

Andrey Chuvilin, Stefan Merkens, Christopher Tollan, and Marek Grzelczak.

A daytime radiative cooling cementitious composite (DRCCC)

EP23382854.0

Jorge S. Dolado, Guido Goracci, Andrés Ayuela, Silvia Arrese-Igor, Miguel Beruete, Iñigo Liberal, Carlos Lezaun, Alicia Torres, José Manuel Pérez-Escudero, Juan José Gaitero, Achutha Prabhu, Edduardus Koenders, Christophe Mankel, Neven Ukraincyk, Ignacio Peralta, Matteo Cagnoni, Federica Capelluti, Antoine Sylvander, Denis Barbier, Karen Allacker, and Nick Adams.

Composition for removing pharmaceuticals and heavy metals from polluted water

21739369

Javier Martinez Sabando, Francesco. Coin, Gustavo A. Schwartz, and Silvina Cerveny.

EDUCATION

As a joint center which belongs to the University of the Basque Country (UPV/EHU), the training activities at CFM include 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 and post-doctoral researchers training. All these activities are strongly related to and coordinated with the research activities of the different research groups at CFM. In the following we note the main aspects of the training activities at CFM.

POST-DOCTORAL TRAINING

CFM encourages the research groups to hire post-doctoral researchers through internal calls, which support around 2-3 post-doc positions every year. Post-doctoral researchers make extremely valuable contributions to the research activities, but they are at an early stage of their scientific careers, which means that they still need to acquire further research skills to successfully develop their scientific careers at a later stage. Therefore each research group makes an individual follow-up and training program for 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, more than 70 pre-doctoral researchers develop their research fully embedded in the daily life of the research groups in the center.

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

DEFENDED PHD THESES

- **Nanoscale physical properties of polymer thin films for energy applications**

Author: Matteo Sanviti

Supervisors: Daniel Martínez Tong, and Ángel Alegría Loinaz

Group: Polymers and Soft matter

31/01/2023

- **Concentration fluctuations and broadening of the glass transition in dynamically asymmetric mixtures**

Author: Numera Shafquat

Supervisors: Arantxa Arbe Mendez, and Ángel Alegría Loinaz

Group: Polymers and Soft matter

31/01/2023

- **Stacking and their boundaries in few-layer graphene: stability and electronic properties in bi- and trilayer Graphene**

Author: Raul Ignacio Guerrero Avilés

Supervisors: Andrés Ayuela Fernández, and Marta Pelc

Group: Electronic Excitations in Surfaces and Nanostructures

20/02/2023

- **Dynamics of the photo-induced desorption and oxidation of CO on Ru(0001) with different (O, CO) coverages**

Author: Auguste Tetenoire

Supervisors: Maite Alducin Ochoa, and J. Iñaki Juaristi Oliden

Group: Gas/Solid Interfaces

23/03/2024

- **Experimental and theoretical investigation of strong acid hydrates**
Author: Sophie Espert
Supervisors: Arnaud Desmedt (CNRS), and Daniel Sánchez Portal
Group: Modelisation and Simulation
30/03/2023
- **Ab initio study of hydrogen based superconducting compounds at ambient pressure**
Author: Antonella Meninno
Supervisor: Ion Errea Lope
Group: Quantum Theory of Materials
04/04/2023
- **Atomic and molecular structures on a superconducting surface**
Author: Cristina Mier González
Supervisors: Nicolás Lorente Palacios, and Deung-Jang Choi
Group: Quantum Phenomena on Surfaces
04/05/2023
- **Layered transition metal oxides: magnetic properties and excitations**
Author: Mikel Arruabarrena Larrarte
Supervisors: Andrés Ayuela Fernández, and Aritz Leonardo Liceranzu (BCB, UPV/EHU)
Group: Electronic Excitations in Surfaces and Nanostructures
05/05/2023
- **Theoretical description of light emission in the presence of nanoscale resonators: from classical scattering to photon states entanglement and statistics**
Author: Alvaro Nodar Villa
Supervisors: Javier Aizpurua Iriazabal, and Ruben Esteban Llorente
Theory of Nanophotonics
19/05/2023
- **Exploring the frontiers of ferromagnetic insulator/superconductor-based devices: surface science developments to explain mesoscopic properties**
Author: Carmen González Orellana
Supervisors: Maxim Ilin, and Celia Rogero Blanco
Group: Nanophysics Lab
22/06/2023
- **Development of sensors for individual barium ion identification in the context of the NEXT experiment**
Author: Pablo Herrero Gómez
Supervisors: Celia Rogero Blanco, and Francesc Monrabal Capilla (DIPC)
Group: Nanophysics Lab
23/06/2023
- **Optimization of Sol-Gel synthesis parameters for obtaining transparent oxyfluoride glass-ceramics with improved optical properties**
Author: María Eugenia Cruz
Supervisors: Yolanda Castro (Instituto de Cerámica y Vidrio- Universidad Autónoma de Madrid), and Rolindes Balda de la Cruz
Group: Laser Physics and Photonic Materials
28/07/2023

- **Pectin-based adsorbents for remediation of contaminated water with pharmaceutical products and heavy metals**
Author: Javier Martínez Sabando
Supervisor: Silvina Cervený Murcia
Group: Polymers and Soft matter
26/09/2023
- **On the dynamics of polymers and biomolecules through the use of machine learning algorithms**
Author: Claudia Borredon
Supervisors: Gustavo A. Schwartz, and Luis A. Miccio Stefancik
Group: Polymers and Soft matter
25/10/2023
- **Quantum-mechanical study of optical excitations in nanoscale systems: first-principles description of plasmons, tunneling-induced light emission and ultrastrong light-matter interaction**
Author: Unai Muniain Caballero
Supervisors: Rubén Esteban Llorente, and Vyacheslav M. Silkin (DIPC)
Group: Theory of Nanophotonics
08/11/2023
- **Rare-earth-noble-metal surface alloys and its interaction with phthalocyanine molecules**
Author: Rodrigo Castrillo Boderó
Supervisors: Frederik M. Schiller, and Laura Fernández Gómez-Recuero
Group: Nanophysics Lab
13/11/2023
- **Space-time symmetries in classical and quantum electromagnetic scattering theory**
Author: Jon Lasa Alonso
Supervisors: Gabriel Molina Terriza, and Aitzol García Etxarri (DIPC)
Group: Quantum nanophotonics Laboratory
11/12/2023

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 16 pre-doctoral researchers have spent about 2-3 months in some of the best international centers on their to-

pics. This training activity combines aspects of internationalization and excellence, and has been strongly supported by CFM over the last years. The following pre-doctoral researchers benefited from an internship abroad supported by CFM in 2023:

- **Adrian Juan Delgado**
Quantum and Nano-Optics Laboratory in Lausana (Italy)
01/10 - 30/11
- **Alaa Mohammed Idris Bakhit**
BESSY II synchrotron Helmholtz-Zentrum, Berlin (Germany)
01/04 – 30/06
- **Ainara Ruiz Bardillo**
Jülich Forschungszentrum (Germany)
21/08 – 21/11
- **Alberto Hijano Mendizabal**
Jyväskylä University (Finland)
01/03 - 30/04

- **Cristina Macia Castello**
ISIS RAL de Didcot, Oxfordshire (United Kingdom)
22/04 – 22/07
- **Davide Arena**
Institut des Biomolécules Mx Mousseron IBM,
Monpellier Université (France)
18/05 - 04/07
- **Divya Jyoti**
Institute de Physique et Chimie des matériaux of
Strasbourg (France)
15/01 – 15/04
- **Francesco Coin**
Universidad de Buenos Aires (Argentina)
31/03 - 28/06
- **Iker Gómez Vilorio**
NanoSoft Laboratory, Instituto per Processi Chimico-Fisici, Messina (Italy)
01/09 – 30/11
- **Josu Diego López**
Università di Modena (Italy)
11/04 - 30/07
- **Martín Molezuelas Ferreras**
Università Federico II, Naples (Italy)
29/07 – 29/12
- **Mohammad Rahjoo**
TU Darmstadt (Germany)
01/01 – 01/03
- **Paula Angulo Portugal**
Berkeley University (EEUU)
29/03 - 28/06
- **Samuel Kerschbaumer**
Institute of Physics of the Czech Academy of
Sciences, Prague (Czech Republic)
29/05-29/06
- **Xabier Arrieta Aristi**
Institute of Physics of the Czech Academy of Science,
Prague (Czech Republic)
08/05-10/06
- **Zuzana Lawera**
Neurotechnology Center at Columbia University,
New York (EEUU)
15/09 - 31/12

PHD RECRUITMENT FAIR 2023

In 2023, MPC-CFM organized the sixth Recruitment Fair for pre-doctoral research staff as part of the strategic plan to attract new talent. Of the 107 applications (26% female) received, 21 candidates were shortlisted (50% female) for online interviews. During the interviews, the selected candidates had the opportunity to discuss the research projects with the supervisors of the different projects and/or the Evaluation Committee.

After the evaluation, 4 candidates were selected and awarded full scholarships to join an MPC-CFM research group:

- **Manex Alkorta Lopetegui**
Supervisor: Ion Errea Lope
Group: Quantum Theory of Materials
- **Sebastian Jiménez Millán**
Supervisor: Armando Maestro Martín
Group: Polymers and Soft Matter
- **Sebastian Negrete Aragón**
Supervisor: Enrique Ortega Conejero
Group: Nanophysics Lab
- **Sruthibhai Palakkattu**
Supervisor: Sara Barja Martínez
Group: Nanophysics Lab

This selection
process has been
analyzed from
a gender
perspective.

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. 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 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 2023, three graduates were awarded scholarships for the Master in Nanoscience program:

- Iñaki Fernández Tena
- Jaime Blanco Caldevilla
- Pablo Gila Herránz

THESES OF THE NANOSCIENCE MASTER SUCCESSFULLY DEFENDED IN 2023

- **Vibrational dynamics of CO on Pt(111) in and out of thermal equilibrium**
Author: Iñaki Fernández Tena
Supervisors: Maite Alducin Ochoa, and Raul Bombín Escudero (Universitat Politècnica de Catalunya)
- **Characterization of low symmetry ReS₂ flakes for optoelectronic device fabrication**
Author: Lucia Olano Vegas
Supervisors: Luis E. Hueso Arroyo (CIC nanoGUNE), and Beatriz Martín García (CIC nanoGUNE)
- **Structure stabilization in hybrid perovskites. Insights from neutron scattering and simulations**
Author: Pablo Gila Herranz
Supervisors: Kacper Druzicki, and Felix Fernandez Alonso
- **Laser-coupled multielectrode array system for plasmon-driven neuronal stimulation**
Author: Gaizka Otegi López
Supervisor: Marek Grzelczak
- **Molecular mobility in simplified Industrial ternary mixtures for tire applications**
Author: Jaime Blanco Caldevilla
Supervisor: Ángel Alegría Loinaz
- **Ab-initio study of melamine on Cu(100): inelastic electron tunneling spectroscopy and the impact of tautomerization**
Author: Manex Alkorta Lopetegui
Supervisor: Thomas Frederiksen

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. CFM hosted the visit of 7 undergraduate students, and supported the defense of 5 of those.

DEFENDED BACHELOR PROJECTS

- **X-Ray Photoelectron Spectroscopy applied to a fluorescent molecular sensor with atomic sensitivity**
Author: Adelina López Romera
Supervisors: Celia Rogero Blanco, and Elisa Palacios Lidón (Universidad de Murcia)
Group: Nanophysics Lab
- **Active photonic devices based on spintronic-plasmonic metasurfaces**
Author: Ángela Díez
Supervisor: Nerea Zabala Unzalu
Group: Theory of Nanophotonics
- **Synthesis of crosslinked polymers with reversible enamine-type bonds**
Author: Marta Aldecoa Ortueta
Supervisors: Josetxo Pomposo Alonso, Ester Verde Sesto, and Fabienne Barroso Bujans
Group: Polymers and Soft matter
- **Síntesis físico-química de un material bidimensional y su caracterización estequiométrica: PbBr₂ sobre HOPG**
Author: Xabier Guerrero Ricarte
Supervisor: Lucía Vitali
Group: Spectroscopy at Atomic Scale
- **Diseño de liposomas y bicapas lipídicas soportadas sobre sólidos para su uso como sistemas biomiméticos**
Author: Ainhoa López de Uralde Baltasar
Supervisors: Armando Maestro, and Javier Aldazabal Mensa (Tecnun Universidad de Navarra)
Group: Polymers and Soft matter

A blurred background image showing a group of people, likely at a conference or workshop. In the foreground, a woman with blonde hair and glasses is visible on the left, and a man with dark hair and glasses is on the right. The image has a soft, out-of-focus quality with a blue and yellow color overlay.

WORKSHOPS, CONFER- ENCES, SEMINARS & COURSES

CFM scientists have organized or co-organized several international workshops and conferences during 2023. Many of these meetings have been held in close cooperation with the Donostia International Physics Center (DIPC), which is an example of the excellent results brought by the synergistic collaboration between both institutions. These activities improve the impact and relevance of the individual and groups' research outcome dramatically.

Moreover, CFM researchers attended requests to give more than **60 invited and plenary talks** in international conferences, showing their leadership in their respective fields.

The list of conferences, workshops, courses, and seminars organized or co-organized by CFM researchers during 2023 is as follows:

CONFERENCES

International Conference on Science and Technology of Quantum Matter – QUANTUMatter 2023

Organizers: Antonio Correia (Phantoms Foundation), Ricardo Díez Muiño (DIPC, CFM-CSIC), Juan Jose Garcia-Ripoll (IFF-CSIC), Pablo Ordejón (ICN2), Gloria Platero Coello (C Ramón Aguado (ICMM/CSIC), Alejandro Gonzalez-Tudela (IFF-CSIC), Diego Porras (IFF-CSIC), and Alejandro Pozas (UCM).

📍 Madrid

📅 23-25/05/2023

Quantum Phenomena in 2D Matter (QP2DM)

Organizers: Vitaly Golovach (CFM-UPV/EHU, DIPC, Ikerbasque), Michael Zudov (University of Minnesota), and Evgeny Sherman (University of the Basque Country, Ikerbasque).

📍 Miramar Palace (Donostia / San Sebastián)

📅 17-21/07/2023

The Third Spins on Surface Workshop (SoS III)

Organizers: Deung-Jang Choi (CFM-CSIC-UPV/EHU, DIPC, Ikerbasque), and Andreas Heinrich (Center for Quantum Nanoscience, Korea).

📍 Miramar Palace (Donostia / San Sebastián)

📅 11-15/09/2023

AI Photonics 2023

Organizers: Aitzol García-Etxarri (DIPC, Ikerbasque), Javi Aizpurua (DIPC, CFM-CSIC), Cefe López (DIPC, ICMM-CSIC), and David Gacía (ICMM-CSIC).

📍 Carlos Santamaría Centre (Donostia / San Sebastián)

📅 11-14/09/2023

Equality, science and technology. For a paradigm shift

Organizers: Itziar Otegui (CIC nanoGUNE), Idoia Múgica Mendiola (CFM), Mónica Moreno (POLYMAT, Marta Macho (UPV/EHU), Jaime Sagarduy (Achucarro Basque Center for Neuroscience), Lorena Fernández (Universidad de Deusto), Irantzu Llanera (CIC biomaGUNE), Naiara Arri (Elhuyar), Iñigo Alustiza (Ikerbasque), Ainhoa Madariaga (Ikerbasque), Eider Ayuso (communication manager at the congress), Ander Bergara (Emakunde), and Maria Sierra (Emakunde).

📍 Miramar Palace (Donostia / San Sebastián)

📅 23-24/10/2023

WOKSHOPS

Software Carpentry Workshop

Instructors: Iñigo Aldazabal (CFM), Abel Carreras (DIPC), Ainhoa Oliden (UPV/EHU), and David de Sancho (DIPC). Helpers: Mikel Arocena (CFM), Irene Azaceta (CFM), Antoine Patt (CFM), and Rubén Pellicer (CFM).

 CFM

 10, 17, 19 and 27/01/2023

NeIC Coderefinery Workshop

Organizer: Radovan Bast et al. (Nordic e-Infrastructure Collaboration (NeIC)). Local coordinators Iñigo Aldazabal (CFM), and Abel Carreras (DIPC).

 Barriola Center, UPV/EHU (Donostia / San Sebastián)

 21-23 and 28-30/03/2023

Translight: Workshop Bordeaux-San Sebastian on Quantum Nanophotonics

Organizer: Quantum Nanophotonics Laboratory

 CFM

 18-19/12/2023

COURSES

An introduction to quantum computing

Organizers: Yvan Le Borgne (Département Combinatoire et Algorithmique, LABRI, Université Bordeaux & CNRS).

 CFM

 06-08/06/2023

1st MIRACLE Course

Organizer: Jorge Sánchez Dolado (CFM).

 TU Darmstadt

 26-28/04/2023

Rilem Multiscale Modelling Course for Concrete (MMC2)

Organizer: Jorge Sánchez Dolado (CFM).

 CFM

 02-06/10/2023

Summer School on the Calculation of Ionic Quantum and Anharmonic Effects with the Stochastic Self-Consistent Harmonic Approximation

Organizers: Ion Errea (UPV/EHU, Spain), Diego Martínez (CFM, Spain), and Lorenzo Monacelli (EPFL, Switzerland).

 CFM

 26-30/06/2023

SEMINARS

Cylindrical Micro- and Nanowires: From Curvature Effects on Magnetization to Sensing Applications

Manuel Vázquez Villalabeitia (CSIC)

📅 15/02/2023

Unveiling elusive physical phenomena in van der Waals systems via the valley Zeeman effect

Paulo-Eduardo Faria-Junior

📅 05/06/2023

Fully-atomistic light-driven dynamics in plasmonic nanosystems, cavities and interfaces

Franco Bonafe (Max Planck Institute for the Structure and Dynamics of Matter)

📅 02/03/2023

Light-Matter Interaction in Emerging Semiconductors

Shahzada Ahmad

📅 02/06/2023

Semiconductor quantum emitters under light-matter coupling conditions

Victor Krivenkov (CFM)

📅 08/03/2023

Spin Transport through Heavy Metal/Magnetic Insulator Interfaces

Sara Catalano

📅 21/06/2023



QUANTUM BREAKFAST

Starting in 2021, and promoted by CFM researcher Miguel Varga, “The Quantum Breakfast seminar series” intended to be educational in a relaxed atmosphere. They are a great opportunity to gain insight in quantum technologies, as well as to bring together the local community. In 2023, starting in April, they were organized on a monthly base with three or four researchers sharing their experience and knowledge:

📅 JANUARY 27	📅 MARCH 31	📅 APRIL 28
The Anomalous Andreev interferometer Alberto Hijano Mesoscopic Physics Group-CFM Helicity states for classical and quantum communications Jon Laso Alonso Quantum Nanophotonics Lab-CFM On the emission of individual colloidal semiconductor quantum dots Adam Olejniczak Nanomaterials and Spectroscopy Group-CFM	Magnetic impurities on proximitized metals Jon Ortuzar Andrés Nano Imaging group-CIC nanoGUNE Graphene plasmonics Alexey Nikitin 2D Nanophotonics group- DIPC	Phonon anharmonicity and superconductivity in high-pressure hydrides Đorđe Dangić Quantum Theory of Materials-CFM Using adatoms for quantum operations Nicolás Lorente Quantum Phenomena on Surfaces-CFM
📅 MAY 26	📅 JUNE 23	📅 JULY 28
Spectroscopic signature of spin triplet odd-valley superconductivity in two-dimensional materials Tim Kikkeler Mesoscopic Physics Group-CFM The Single Characterization angle method for cylindrical particles Jorge Olmos-Trigo Quantum Nanophotonics Lab-CFM	Quantum Machine learning via variational algorithms Pablo Bermejo Navas Multiverse Computing & Quantum Systems and Technologies Group- DIPC Quantum Nanophotonics with Hexagonal Boron Nitride Igor Aharonovich University of Technology Sydney, Australia	Wireless Microwave Quantum Communication Tasio Gonzalez Raya Basque Center for Applied Mathematics (BCAM) Plexcitonic Systems: Synthesis and Optical Characterization Alba Jumbo Nanomaterials and Spectroscopy group and ColSysChem group-CFM
📅 OCTOBER 27	📅 NOVEMBER 24	
Special pre-Halloween talk: Current development of “Frankenstein” methods in Quantum Chemistry Aarón Rodríguez-Jiménez Molecular Electronic Structure Group-DIPC Exploring Quantum Chemistry with Variational Quantum Eigensolvers Abel Carreras Molecular Electronic Structure Group-DIPC and Multiverse Computing	The molecular magnetic response as a quantification of electronic delocalization: A look at three-dimensional aromaticity Mesías Orozco Ic Quantum Chemistry Development Group-DIPC Characterization of molecular magnetism and its use in potential spin-qubits Antonio Cebreiro Molecular Electronic Structure Group-DIPC	

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 Pomeraniec (CFM), DIPC and CFM have launched a full program covering issues like stress management, time and career management or transformative leadership. **55 researchers** joined the three courses organized in 2023 in the framework of this program.

Emotional Well-being in Science

Sofia Facal (Skills for Science and Industry)

 DIPC

 10, 19, and 24/05/2023

The Emotional Well-being in Science training was designed to provide predoctoral researchers with tools and strategies to manage the emotional challenges of academia. The three sessions covered topics such as understanding emotional distress and mental health issues, building resilience and self-care, and creating a supportive environment, through interactive activities, case studies, and group discussions.

Session 1	Session 2	Session 3
Understanding Emotional Well-being in Academia • Introduction & Understanding the emotional challenges of being a PhD student • Identifying signs of emotional distress and mental health issues • Strategies for coping with stress and anxiety • Imposter syndrome	Building Resilience and Self-care • Building resilience to handle academic and personal challenges • Knowing and developing helpful routines for emotional and physical well-being • Strategies for maintaining work-life balance	Creating a Supportive Environment • Strategies for building a supportive network • - Importance of good communication skills to handle difficult situations • - Building a culture of well-being in academia

Time and Career Management

Sofia Facal (Skills for Science and Industry)

 CFM

 23-25/10/2023

This training aimed to provide a comprehensive and interactive learning experience for predoctoral researchers in scientific careers, helping them enhance their time management skills and navigate the diverse career paths available, whether within academia or beyond. Each session included a mix of presentations, practical exercises, and opportunities for discussion and engagement with experts in the field.

The content of the workshop included:

- Develop effective time management strategies
- Gain the skills to prioritize tasks and set achievable goals
- Learn how to plan and organize your work for optimal results
- Dealing with Procrastination
- The Changing Landscape of Scientific Careers
- Creating a personalized career plan to align with your aspirations
- Navigating the Academic Job Market
- Exploring Career Opportunities in Technology Centers
- Transitioning to Industry: Application Process
- Preparing your materials: CV industry vs CV academia
- Interview Preparation

Navigating the Research Seas: Transferable Skills for PIs

Sofia Facal (Skills for Science and Industry)



16, 23 and 30/11/2023

This training program was designed to address the need for soft skills development among Principal Investigators (PIs). The role of a PI goes beyond technical expertise, as they are responsible for shaping the direction of their research teams and fostering a culture of excellence. As emphasized by the questionnaire elaborated for PI's in CFM and DIPC community, good leadership skills are indispensable for avoiding problems within a group and enhancing overall productivity.

Three sessions were arranged that align with the various phases of group dynamics, enabling PIs to have tips and tools to tackle how to form, navigate challenges, and optimize their research teams. The course explored the critical aspects of leadership, from forming a good-performing group to handling diversity and conflicts, and finally, fostering productivity and motivation within the research team.

Session 1	Session 2	Session 3
Forming the group • Leadership styles, how to combine them • Group dynamics: phases and what is needed in each stage • Establishing a clear vision and values for your research group. • Strategies for attracting, onboarding, and retaining the right team members for your group.	Group Storming - Cultivating Communication and collaboration • Effective communication skills in a diverse multicultural environment. • Feedback: transforming critics into constructive contributions • Conflict resolution strategies for maintaining balance within the group. • Navigating diverse perspectives and fostering collaboration.	Group Norming - Keeping Motivation and working effectively • Time management techniques. • Delegation and empowerment strategies. • Techniques for keeping the research team motivated and engaged, ensuring sustained • Productivity and collaboration in a good environment.

COMPETITIVE FUNDING FOR RESEARCH PROJECTS

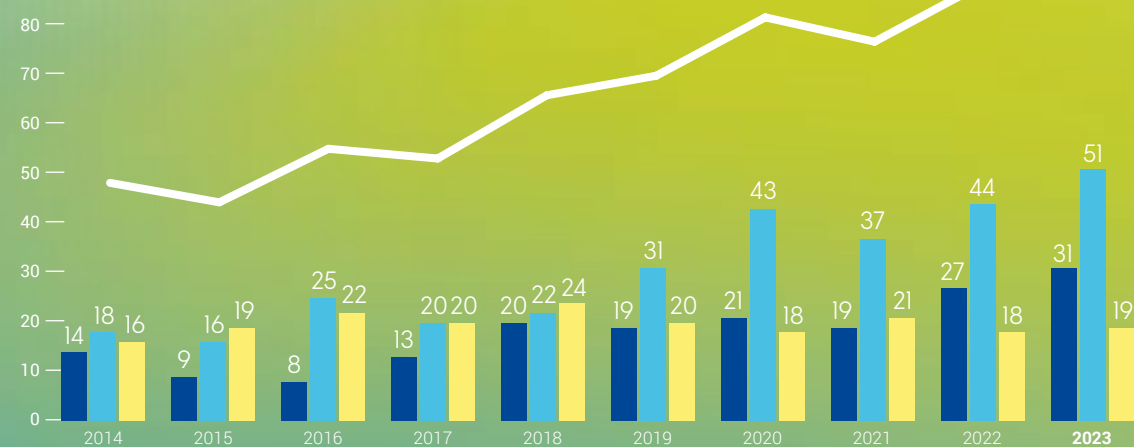
Boosting the participation of researchers in competitive public projects is a strategic priority of our center. Particularly, participating in collaborative projects is key to building the basis of competitive networks capable of facing the current and future challenges in advanced materials science in a synergetic way. Research groups are very active in submitting applications to local, national and international calls launched by the principal funding agencies. As a result, the number of ongoing competitive projects has significantly increased in the last years. Regarding international projects, it is worth noting the intense participation

of researchers in EIC (European Innovation Council) Pathfinder calls and ERC (European Research Council) calls, both in the framework of Horizon Europe. The projects and networks ongoing during 2023 (a total of 101 projects/networks) are listed below according to the source of competitive funding.

Regarding public funds for research activity, the center obtained more than 8.8 million euros in 2023, including funds provided by the Basque Government in the framework of the IKUR strategy and BERC 2022-2025 contribution for 2023.

Research projects and networks	Competitive public funds obtained in 2023
BASQUE	2491 518,61 €
SPANISH MINISTRY	2089397,00 €
INTERNATIONAL	2915161,71 €
MPC-BERC	1 383849,00 €
Total	8879926,32 €

100 — Ongoing projects
and networks



BASQUE RESEARCH PROJECTS AND NETWORKS

- EJ/GV, Hezkuntza Saila/Departamento de Educación, IKERTALDE 2022, Grupo Consolidado IT1526-22

Q-NANOFOTONIKA: Nanofotónica para la identificación y desarrollo de nuevos procesos y aplicaciones en espectroscopías moleculares, microscopía de campo cercano y tecnologías cuánticas.

PI: Javier Aizpurua Iriazabal

Co-PI: Nerea Zabala Unzalu

- EJ/GV, Hezkuntza Saila/Departamento de Educación, IKERTALDE 2022, Grupo Consolidado IT1566-22

Polimeros y materia blanda / Polymers and soft matter (PSMG)

PI: Arantxa Arbe Méndez

Co-PI: Angel Alegria Loinaz

- EJ/GV, Hezkuntza Saila/Departamento de Educación, IKERTALDE 2022, Grupo Consolidado IT1569-22

Grupo de Fisicoquímica de Superficies y Nanoestructuras.

PI: Iñaki Juaristi Oriden

- EJ/GV, Hezkuntza Saila/Departamento de Educación, IKERTALDE 2022, Grupo Consolidado IT1591-22

Nanophysics Lab San Sebastian: desde la ciencia de superficies a los dispositivos.

PI: Celia Rogero Blanco

Co-PI: José Enrique Ortega Conejero

- EJ/GV, Hezkuntza Saila/Departamento de Educación, IKERTALDE 2022, Grupo Consolidado IT1707-22

From protein folding prediction to personalized medicine with artificial intelligence.

PI: Aitor Bergara Jauregi

Co-PI: Álvaro Villarroel (no CFM)

- EJ/GV, Hezkuntza Saila/Departamento de Educación, IKERTALDE 2022, Grupo Consolidado IT1453-22

FunThEMaS: Fundamental Theoretical and Experimental Materials Science.

Partner: Lucia Vitali

BASQUE RESEARCH PROJECTS AND NETWORKS

- EJ/GV, Hezkuntza Saila/Departamento de Educación, IKERTALDE 2022, Grupo Consolidado IT1527-22

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

Partner: Ion Errea

- EJ/GV, Ekonomiaren Garapen, Jasangarritasun eta Ingurumen Saila/Departamento de Desarrollo Económico, Sostenibilidad y Medio Ambiente, ELKARTEK 2022, Programa de Ayudas a la Investigación Colaborativa en áreas estratégicas (KK-2022/00062)

QFIRST: Dispositivos en Tecnologías Cuánticas

PI: Gabriel Molina Terriza

- EJ/GV, Hezkuntza Saila/Departamento de Educación, Proyectos de Investigación Básica y/o Aplicada 2023-2025 (PIBA), PIBA_2023_1_0006

Desarrollo y caracterización de materiales micro-nano-estructurados activados con colorantes orgánicos y/o tierras raras para la elaboración de láseres aleatorios con aplicaciones optoelectrónicas.

PI: Rolindes Balda de la Cruz

- EJ/GV, Hezkuntza Saila/Departamento de Educación, Proyectos de Investigación Básica y/o Aplicada 2023-2025 (PIBA), PIBA_2023_1_0054

Design of intelligent drug delivery systems based on polymer nanoparticles for overcoming cellular membrane barriers.

PI: Armando Maestro

- EJ/GV, Hezkuntza Saila/Departamento de Educación, 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

- EJ/GV, Hezkuntza Saila/Departamento de Educación, 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

BASQUE RESEARCH PROJECTS AND NETWORKS

- EJ/GV, Hezkuntza Saila/Departamento de Educación, Ayudas para la adquisición de equipamiento científico 2023 (INKER), EC_2023_1_0010

Electron spin resonance scanning tunneling microscope (ESR-STM).

PI: Deungjang Choi

- EJ/GV, Hezkuntza Saila/Departamento de Educación, Ayudas para el Programa Predoctoral de Formación de Personal Investigador No Doctor correspondiente al curso 2022-2023

5 ayudas para contratación de personal investigador predoctoral

- Lanbide - Servicio Vasco de Empleo, Programa INVESTIGO (2022/IKER/000022)

Gestión de sistemas de supercomputación y Servicios TIC avanzados en el ámbito I+D+i.

- Lanbide - Servicio Vasco de Empleo, Programa PRIMER EXPERIENCIA (2022/PEX/000014)

Técnico/a de sistemas TIC.

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Fellows Gipuzkoa – Atracción 2023, 2023-FELL-000014-01

Ingeniería de arquitecturas mesoporosas a través del autoensamblaje de copolímeros de bloque para la fabricación de biosensores electroquímicos.

Beneficiary: Alberto Álvarez

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Fellows Gipuzkoa – Retención 2023, 2023-FELL-000013-01

Nanopartículas fototérmicas de oro biofuncionalizadas para su retención en la membrana de neuronas y evocar potenciales de acción.

Beneficiary: Ane Escobar Fernández

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Fellows Gipuzkoa – Atracción 2022, 2022-FELL-000009-01

Descripción teórica de reacciones térmicas en superficies.

Beneficiary: Ane Escobar Fernández

BASQUE RESEARCH PROJECTS AND NETWORKS

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa QUANTUM 2023, 2023-QUAN-000022-01

Quantum correlations in nanostructures for quantum applications.

Proyecto I+D con la Fundación Donostia International Physics Center (DIPC)

PI: Marek Grzelczak

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa QUANTUM 2023, 2023-QUAN-000027-01

Líquidos y Diamantes. Resonancia magnética nuclear de bolsillo.

Proyecto I+D con la empresa Microliquid y Fundación Tekniker

PI: Gabriel Molina Terriza

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa QUANTUM 2023, 2023-QUAN-000029-01

Quantum register based on molecular spins and graphene nanostructures.

Proyecto I+D con el CIC Nanogune

PI: Frederik Schiller

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa QUANTUM 2022, QUAN 36/2022

Desarrollo y fabricación de los circuitos eléctricos híbridos semiconductor-superconductor para los qubits.

Proyecto I+D con la empresa Fagor Electronics

PI: Celia Rogero Blanco

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa Coopera 2022, 2022-IZEN-10

Ellas investigan VI: Afrikar emakumezko ikertzaile batek egonaldi bat egin dezan MPCn / Ellas investigan VI: Estancia de investigación en el MPC de una investigadora africana.

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2023-RED2023, Proyectos Next, 2023-CIEN-000077-01

PEMA: Propiedades electrónicas y magnéticas de metales escasos, sus óxidos y materiales alternativos.

PI: Frederik Schiller

BASQUE RESEARCH PROJECTS AND NETWORKS

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2023-RED2023, Proyectos de I+D, 2023-CIEN-000069-01

PEMA: Propiedades electrónicas y magnéticas de metales escasos, sus óxidos y materiales alternativos.

PI: Jon Maiz

- Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2022-RED2022, Proyectos de I+D, 2022-CIEN-000017-01

Superredes de materiales de van der Waals bidimensionales para sensores optoelectrónicos y magnéticos.

PI: Lucia Vitali, Deungjang Choi

- Donostia Sustapena/Fomento San Sebastián – Mujeres Investigadores 2022

Synthesis and electronic structure of one-atom-thick hexagonal boron nitride on curved crystals: toward boron nitride nanostripes.

Beneficiary: Alaa Mohammed Idris Bakhit

- Euskampus Fundazioa, LTC Green Concrete: Joint Transborder Laboratory for the development of more sustainable production processes and materials for cement composites

Co-coordinator: Jorge S. Dolado

- Euskampus Fundazioa, LTC TRANSLIGHT: Joint Transborder Laboratory in Light sciences and Photonics

Co-coordinator: Javier Aizpurua Iriazabal

- Euskampus Fundazioa, LTC QuantumChemPhys: Joint Transborder Laboratory in Theoretical Chemistry and Physics at the Quantum Scale

Co-coordinator: Ricardo Díez Muiño

SPANISH RESEARCH PROJECTS AND NETWORKS

- **Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-137363OA-I00**

NeuroGold: Nanoestructuras de oro fototérmicas para modular la actividad neuronal Photothermal gold nanostructures for neural activity modulation.

PI: Ane Escobar Fernández

- **Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-136392NA-I00**

ArtEMis: Impulsando la Optimización de Ensamblajes Peptídicos Supramoleculares como Matrices Extracelulares Artificiales.

PI: Ivan Sasselli Ramos

- **Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-141017OB-I00**

PREST: Data-Driven Approach for Accelerating Pulsed Plasmonic Catalysis.

PI: Marek Grzelczak

- **Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-138210NB-I00**

MAPEVDW: Magnetism, electronic properties and epitaxial growth of monolayers of non-centrosymmetric two-dimensional van der Waals materials.

PI: Mikhail Otrokov

- **Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-137845NB-C22**

Photonic Metaconcrete with Photothermoelectric capacity.

PI: Jorge Sánchez Dolado

- **Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-139230NB-I00**

EIEEDyNaCoS: Exploring the Interplay of Electronic Excitations and Dynamics in Nanostructures and Complex Systems.

PI: Andrés Ayuela Fernández

SPANISH RESEARCH PROJECTS AND NETWORKS

- Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-140163NB-I00

TADEO: Theory and Applications of complex gas/surface Dynamics in highly Excited enviroNments.

PI: Maite Alducin Ochoa

- Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-140845OB-C65

ChemSense: Chemical, electronic and optical characterisation of atomically precise molecular architectures for sensing applications.

PI: Martina Corso

- Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-143268NB-I00

HeliForces: Controlling optical forces with helical beams.

PI: Gabriel Molina Terriza

- Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-139579NB-I00

QuEVEDO: Tratamiento cuántico de la interacción de excitones y vibraciones moleculares con nanoresonadores ópticos: fluorescencia, dinámica electrónica ultrarrápida y optomecánica.

PI: Ruben Esteban Llorente

- Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-142861NA-I00

SUPERTRANS: Propiedades vibracionales complejas a partir de cálculos ab initio: superconductividad de alta temperatura, transiciones de fase y transporte térmico.

PI: Ion Errea Lope

- Proyectos de I+D+i de Generación de Conocimiento 2022 (PID2022), PID2022-137685NB-I00

CompuMaBo: Metodologías Computacionales para Problemas de Muchos Cuerpos en Física de la Materia Condensada: Vibraciones, Magnetismo y Alta Correlación.

PI: Andrés Arnau Pino

SPANISH RESEARCH PROJECTS AND NETWORKS

- **Proyectos de I+D+i de Generación de Conocimiento 2021 (PID2021), PID2021-124080OB-I00**

TESEO: Diseño y caracterización teórica de nuevos materiales sostenibles para iluminación y la producción de energía solar.

PI: Pedro Braña Coto

- **Proyectos de I+D+i de Generación de Conocimiento 2021 (PID2021), PID2021-123438NB-I00**

DYNANET: Redes Dinámicas en Materia Blanda: De las Moléculas Pequeñas a los Polímeros Complejos.

PIs: Angel Moreno Segurado, Josetxo Pomposo Alonso

- **Proyectos de I+D+i de Generación de Conocimiento 2021 (PID2021), PID2021-127917NB-I00**

MAMI: Moléculas como Impurezas Magnéticas para tecnologías cuánticas.

PIs: Deungjang Choi, Nicolás Lorente Palacios

- **Proyectos de I+D+i de Generación de Conocimiento 2021 (PID2021), PID2021-129054NA-I00**

BIOINTER: Diseño racional de interfases biológicas: de las cuestiones fundamentales a las aplicaciones en la administración de fármacos.

PI: Armando Maestro Martín

- **Proyectos de I+D+i de Generación de Conocimiento 2021 (PID2021), PID2021-123438NB-I00**

HigherOrder: Teoría ab initio de respuestas de transporte y ópticas de orden superior en cristales.

PIs: Ivo Souza, Stepan Tsirkin

- **Proyectos Estratégicos Orientados a la Transición Ecológica y a la Transición Digital 2021, Tipo B individual, TED2021-129457B-I00**

Materiales metaestables y activos basados en el carbono para el almacenamiento y gestión de energías limpias: nuevas estrategias físico-químicas (MACMAT).

PIs: Félix Fernández Alonso, Pedro Braña Coto

SPANISH RESEARCH PROJECTS AND NETWORKS

- **Proyectos Estratégicos Orientados a la Transición Ecológica y a la Transición Digital 2021, Tipo A individual, TED2021-130107A-I00**

Polímeros y Nanocompuestos Altamente Polares para Almacenamiento de Energía: desde el Diseño y la Síntesis hasta la Caracterización Estructural y Dinámica (POLARAGE).

PIs: Jon Maiz Sancho, Ester Verde Sesto

- **Proyectos Estratégicos Orientados a la Transición Ecológica y a la Transición Digital 2021, Tipo B coordinador, TED2021-132074B-C31**

Hormigón fotónico para soluciones medioambientales (PCES).

PIs: Jorge Sánchez Dolado, Juan José Gaitero Redondo (TECNALIA)

- **Proyectos Estratégicos Orientados a la Transición Ecológica y a la Transición Digital 2021, Tipo B subproyecto, TED2021-132074B-C32**

Propiedades de Respuesta en Hormigones Fotónicos para Soluciones (RePro-PCES).

PI: Andrés Ayuela Fernández

- **Proyectos Estratégicos Orientados a la Transición Ecológica y a la Transición Digital 2021, Tipo B subproyecto, TED2021-130292B-C42**

Desarrollo de nuevos materiales para dispositivos cuánticos (NEMATODE).

PIs: Celia Rogero Blanco, Sebastian Bergeret Sbarbaro

- **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

SPANISH RESEARCH PROJECTS AND NETWORKS

- **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.

PIs: Sebastián Bergeret Sbarbaro, 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.

PIs: Sara Barja Martínez, Frederik Michael Schiller

- **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.

PIs : Silvina Cervený Murcia, Gustavo A. Schwartz Pomeranec

- **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.

PIs: Maite Alducin Ochoa, Ricardo Díez Muiño

SPANISH RESEARCH PROJECTS AND NETWORKS

- Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-105488GB-I00

2EDiSNa - Excitaciones electrónicas y dinámicas en superficies y nanoestructuras.

PIs: Andrés Ayuela Fernández, 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.

PIs: Javier Aizpuru Iriazabal, Rubén Esteban Llorente
- Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-103910GB-I00

VIMAGSOC - Vibraciones y magnetismo en sistemas nanoscópicos con acoplamiento spin-órbita.

PIs: Andrés Arnau Pino, 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.

PIs: Marek Grzelczak, 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.

PIs: Martina Corso, 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.

PIs: Daniel Sánchez Portal, Arantzazu García Lekue (DIPC, Ikerbasque)

SPANISH RESEARCH PROJECTS AND NETWORKS

- Consolidación Investigadora 2022 (CNS 2022), CNS2022-136171
Low-Dimensional Halide Perovskite for optoelectronics applications (PEROPS).
PI: Samrana Kazim
- Redes Investigación 2022 - Red Temática, RED2022-134508-T
CAT&SCALE: (Foto-) Electrocatalisis: de la escala atómica a dispositivos avanzados.
PI, Network Coordinator: Sara Barja Martínez
- Ayudas Juan de la Cierva (JdC) 2021, FJC2021-047090-I
Chiral Anapoles / Fuentes quirales no radiantes.
PI: Gabriel Molina Terriza
Beneficiary: Jorge Olmos Trigo
- Ayudas Juan de la Cierva (JdC) 2021, FJC2021-047710-I
Non-equilibrium self-assembly and catalysis with metal nanoparticles.
PI: Marek Grzelczak
Beneficiary: Anish Rao
- Ayudas Ramón y Cajal (RyC) 2021, RYC2021-031705-I
Advanced materials for spin- and opto-electronics.
PI: Marco Gobbi
- Ayudas Ramón y Cajal (RyC) 2021, RYC2021-033294-I
Amphiphilic peptides for the development of supramolecular polymers.
PI: Ivan Sasselli Ramos
- Ayudas Ramón y Cajal (RyC) 2017, RYC-2017-21931
Novel physical phenomena in two-dimensional materials.
PI: Sara Barja Martínez
- Ayudas para Personal Técnico de Apoyo (PTA) 2021, PTA2021-021175-I
Apoyo técnico al laboratorio del grupo Polymers and Soft Matter para la especialidad de cromatografía líquida para la caracterización de materiales del CFM - Centro Mixto CSIC-UPV/EHU
Lab Technician: Isabel Asenjo Sanz

SPANISH RESEARCH PROJECTS AND NETWORKS

- Ayudas para Personal Técnico de Apoyo (PTA) 2021, PTA2021-020084-I
Apoyo técnico al laboratorio del grupo Ceramic and Cement-based Materials para el desarrollo de Photonic Metaconcrete y Thermoelectric Concrete del CFM - Centro Mixto CSIC-UPV/EHU.
Lab Technician: Guido Goracci
- Ayudas para 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
- Ayudas para 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
- CSIC, I-LINK+2021, Colaboración Científica Internacional, LINKA20407
Hybrid Nanomaterials for Neuronal Photostimulation.
PI: Marek Grzelczak
- CSIC, Fondo de Apoyo a los Servicios Científico Técnicos (FAS) 2023, FAS2023_056
Detector de fugas con helio.
CSIC, CONEXIONES 2023, Creación de redes de colaboración en el área de la biología computacional y bioinformática
PI: Pedro Braña Coto.
- CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2019, 2023AEP007
FunMolSys: On-Surface Synthesis of Functional Molecular Systems (PID2019-107338RB-C63).
PI: Martina Corso
- CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2019, 2023AEP085
BRIDGE: Cerrando la brecha entre los polímeros sintéticos y los biopolímeros: modelando el comportamiento de biopolímeros a través de los polímeros sintéticos (PID2019-104650B-C21).
PI: Silvina Cervený Murcia

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

- ERC Starting Grant (ERC-2018-StG), GA 802533

SuperH – Discovery and characterization of hydrogen-based high-temperature superconductors.

PI: Ion Errea Lope

- 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-2021-StG), GA 101040193

COSAS - Controlling oxygen selectivity at the atomic scale.

PI: Sara Barja Martínez

- 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

- 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 01-2016-2017), GA800923**

SUPERTED - Thermoelectric detector based on superconductor-ferromagnet heterostructures.

PI: Sebastián Bergeret Sbarbaro

Co-PI: Celia Rogero Blanco

- **HORIZON EUROPE Pathfinder Open (HORIZON-EIC-2021-PATHFINDEROPEN-01-01) ESiM: Energy Storage in Molecules.**

PI: Nicolas 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

- **HORIZON EUROPE Cluster 5 (HORIZON-CL5-2021-D3-03), GA 101084348**

NATURSEA-PV: Novel eco-cementitious materials and components for durable, competitive, and bio-inspired offshore floating PV substructures.

PI: Jorge Sánchez Dolado

- **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

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

- **MSCA Postdoctoral Fellowship (HORIZON-MSCA-2022-PF-01), GA 101106809**
CavityMag: Cavity quantum electrodynamics control of magnetic phases in twisted van der Waals heterostructures.
PI: Angel Rubio Secades
- **MSCA Doctoral Networks (HORIZON-MSCA-2021-DN-01), GA 101072964**
QLUSTER: Quantum and Classical Ultrasoft Matter.
PI: Angel Moreno Segurado
- **COST Action 2021, CA20116**
OPERA - European Network for Innovative and Advanced Epitaxy
Management Committee Member: Sara Barja Martínez
- **COST Action 2017, CA17139**
EUTOPIA - European Topology Interdisciplinary Action.
Management Committee Member: Ángel Moreno Segurado
- **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
- **ONR Global basic and applied scientific research grant (N62909-22-1-2031)**
Microspherical Superlens windows to the quantum world.
PI: Yury Rakovich

TRANSFER OF KNOWLEDGE

Despite being a fundamental research center, the CFM is committed to providing access to all the knowledge and technologies resulting from its scientific activity to have an impact on industry and society. A technology transfer strategy has been developed, generating basic knowledge on advanced materials in order to be used by local and international private initiatives that involve industrial partners, from large international corporations to SMEs, as well as Technology Centers and Cooperative Research Centers.

The portfolio of contracts and collaboration agreements with different companies or entities has been very productive during 2023. Some examples of the partners involved are:



Climate-KIC (EU climate innovation initiative)
Knowledge and innovation community (KIC), working to accelerate the transition to a zero-carbon, climate -resilient society.



Cadarsó (Gipuzkoa)
Specialists in re-carburizing additives for metallurgy



Graphenea (Donostia – San Sebastián)
High quality graphene for industrial applications



Fagor electronics (Gipuzkoa)
Desarrollo y fabricación de circuitos eléctricos híbridos semiconductor-superconductor para qubits



HighFinesse
Knowledge exchange and student internships and courses



SIMUNE ATOMICS L.T.D.
Development of software tools to improve the capabilities and the analysis of data computed with the SIESTA/TranSIESTA package



Považská cementáreň (Slovakia)
Study of hydrated cement pastes



Baskrete cross-border initiative
Concrete science and technology



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



MicroLiquid
R&D collaboration on developing a prototype for compact nuclear magnetic resonance



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



Kutxa Fundazioa
Promoting scientific cultural activities, such as “Que sabemos de...”, “Vidas científicas”, “Fotciencia” and more.

CFM also focuses on the transfer of technology to the Basque industrial network within the framework of the ELKARTEK program of the Department of Industry of the Basque Government (EJ/GV), a program that pursues the generation of fundamental knowledge in specific strategic areas of interest to Euskadi by promoting collaboration between research centers and the industrial fabric. During the year 2023, the center has had a current ELKARTEK project (QFIRST) and has presented several proposals for collaborative projects with companies to the 2023 ELKARTEK call. Three (3) Gipuzkoa QUANTUM projects have also been obtained

from the provincial council, focused on applied research in quantum technology. One of them is led by the company MicroLiquids, with the MPC as a specialist entity.

Technology Centers and Cooperative Research Centers (CIC), such as Tecnalia, AZTI, Tekniker, Cidetek, CEIT and CIC nanoGUNE, regularly collaborate with MPC-CFM within the framework of the ELKARTEK program. In addition, MPC-CFM is part of the Basque BASKRETE Energy network, in which UPV/EHU, Donostia International Physics Center (DIPC), POLYMAT and Tecnalia also participate.

SCIENCE & SOCIETY

The goal of the CFM's Science and Society program is to bridge the gap between science and the public, to enhance public awareness and appreciation of science, and foster a more informed and scientifically literate society, encouraging more active and meaningful participation in scientific research and innovation.

The efforts at CFM have been devoted to achieve mainly three objectives:

- Spreading scientific culture
- Inspiring scientific vocation
- Mainstreaming gender equality in all the activities organized.

Moreover, at CFM we are proud to have a strong community of volunteers ready to spread the message; CFM appreciates the effort and encourages all the scientific staff to join the team, offering training on all the activities organized to those participating.

Over the years, CFM has implemented a comprehensive scientific outreach program, and during 2023 more than 70 activities and events were organized, many of them in collaboration with other institutions.

#scienceandsociety

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



+ 70

activities and events, many of them in collaboration with other institutions

+ 12 500
participants

+ 3 200
views of the virtual contents

+ 40

researchers of CFM's staff (50% women)

THANKS

Culture, Vocation, Gender perspective and Diversity: We do care

Including the **gender and diversity perspective** in all the activities organized is a commitment acquired by CFM and is materialized as follows:

- Maximizing the visibility of our women researchers
- Promoting the awareness on the situation
- Ensuring the gender balance in the talks organized
- 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.

In 2023 this successful program reached more than **750 students** from **18 different schools** that had the chance to interact with more than **20 professionals** from DIPC and CFM. Moreover, the opportunity to participate in the online visits turned out to be a great way to reach schools from further territories like Biscay and small villages that usually could not travel to attend the face to face visit.

The video collection of the premises visited virtually is available on our YouTube channel:

- **Polymer synthesis lab at CFM**
- **Dielectric spectroscopy lab at CFM**
- **Nanophysics lab at CFM**
- **Quantum Nanophotonics lab**

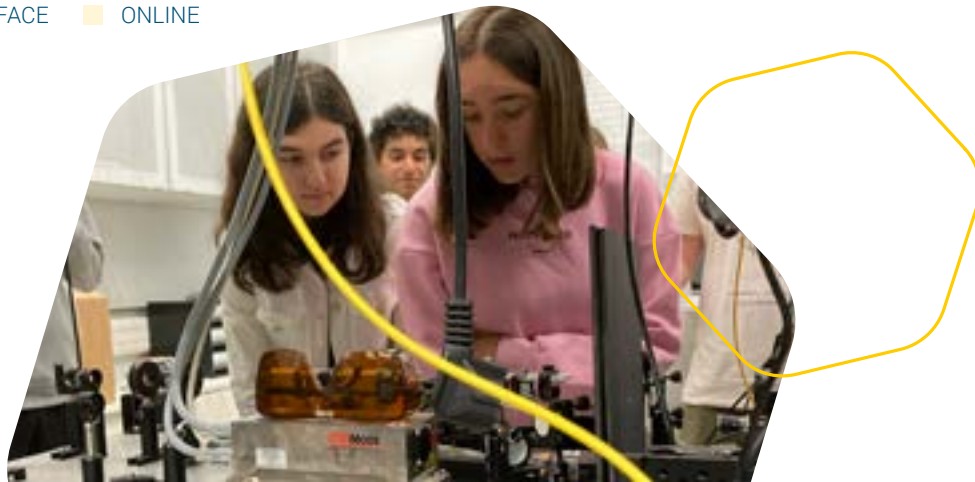


Available at
[CFM's YouTube channel](#) or
scanning this
code

In addition to this visits, since 2021, CFM joined the EGOKITU program. EGOKITU offers young students in the last years of their high school training the possibility to participate in a summer science camp at the UPV/EHU. The Faculty of Chemistry of Donostia / San Sebastián has joined this program for years, offering an immersive experience to two group of students over two weeks that now includes the visit to DIPC and CFM.

JANUARY 27 Laskorain Ikastola	FEBRUARY 10 Emakumeak Zientzian Lauro Ikastola La Anunciata Ikastetxea La Salle kastetxea ORIXE BHI Ballonti BHI Abadiño BHI Soraluze BHI Txintxirri Ikastola	MARCH 17 Toki Ona BHI (Bera)	APRIL 21 Colegio Americano de Bilbao Saturnino de la Peña Facultad de Informática	
JUNE 27 EGOKITU	JULY 4 EGOKITU	NOVEMBER 17 San Ignacio Jesuitak Donostia La Anunciata Ikastetxea	DECEMBER 1 Politeknika Txorierrri	DECEMBER 15 Jesuitak Indautxu Koldo Mitxelena BHI

■ FACE TO FACE ■ ONLINE



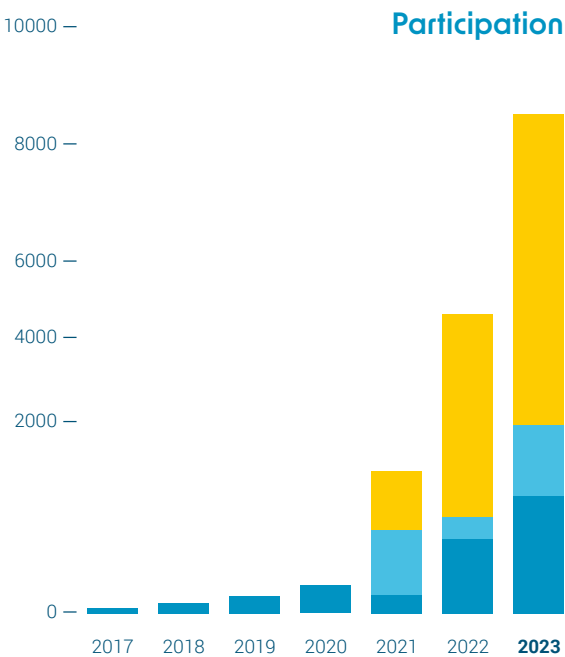
EMAKUMEAK ZIENTZIAN 2023

emakumeakzientzian.eus

8-17/02/2023

Since its inception in 2017 *Emakumeak Zientzian* initiative has evolved into a powerful coalition of different research centers and science institutions, consolidating an unprecedented network and workforce. In 2023 this nonstop wave expanded to Bizkaia reaching **24 entities**, gathering more than 250 volunteers actively participating in the comprehensive program that aimed at all the public, including teenager women, school kids, elder women (above 55), and also the scientific community.

CFM together with CIC nanoGUNE, POLYMAT, CIC biomaGUNE, Achucarro, and Deusto University assumed the coordination of the initiative supported by Gipuzkoa and Bizkaia Provincial Councils, Fomento DSS and Ikerbasque, among other major sponsors.



- Exhibits
- Streaming
- Face to face

For the benefit of society as a whole

54
Activities

+ 8 500
attendees

250
Volunteers

24
research centers and science-related institutions

55 000
of funding



The main objectives remain to be:

- Make visible the activity of women in science
- Break with the typically masculine roles attributed to scientific-technical activities
- Encourage the choice of scientific careers among girls and adolescents.

ERTZAK (edges)

In addition, this year, the organisation wanted to focus on the importance of sharing a joint responsibility between women and men when it comes to promoting equal access and professional development for everyone. A special appeal was made and everyone was invited, regardless of their gender, identity, origin, profession or age, to take part in the activities.

With this goal in mind, Janus Lester, the artist, predoctoral researcher at CFM, and ally of Emakumeak Zientzian, composed a hymn of the cause, to give a cheerful rhythm to the initiative, and also to reach out new allies to share responsibilities: "eman, hartu eskua; egin, utzi lekua..." (give, take the hand, make room). The hymn "Ertzak" is available in the main music platforms, as well as in the YouTube channel of Emakumeak Zientzian.



Listen to the single scanning this code



DSS WEEK INN and EMAKUMEAK ZIENTZIAN

Women scientists of yesterday and today

📍 29/11/2023

📅 Plenary Hall of the San Sebastian City Hall

CFM and Emakumeak Zientzian regularly collaborate in the Innovation Week “Donostia WeekINN” that Fomento of San Sebastian organizes every year. In 2023, this collaboration was materialized in the event “Women scientists of yesterday and today”.

Five women scientists working in research centers in Gipuzkoa took the stage of the Plenary Hall of the San Sebastian City Hall to talk about the research in which they are immersed and pay tribute to some of the most pioneering women scientists in history through the story of their fascinating lives and scientific contributions.



ELIXABETE REZABAL ASTIGARRAGA

Paying tribute to Dorothy Crowfoot Hodgkin

AMAIA ITURROSPE IBARRA (CFM)

Paying tribute to Marie-Anne Pierrette Paulze

RAQUEL RUIZ HERNÁNDEZ

Paying tribute to Rachel Carson

ANA ÁLVAREZ YENES (NANO GUNE)

Paying tribute to Stephanie Kwolek

OLATZ PEREZ DE VIÑASPRE

Paying tribute to Karen Spärck Jones

PINT OF SCIENCE

pintofscience.com

📍 Donostia / San Sebastián

📅 22-24/05/2023

The “Pint of Science” festival aims to deliver interesting and relevant talks on the latest science research in a really informal format: they take place in bars and pubs. The goal is to provide a platform, which allows to discuss research with the people who carry it in a friendly environment. Organized yearly by CIC biomaGUNE, since 2018, CFM supports this festival that fills up our city with science. Cheers!!!

In the framework of this festival, in 2023, three CFM researchers participated with the following talks:

Construyendo nano-sistemas con oro y moléculas

Alba Jumbo Nogales

22/05/2023

La edad del oro de la neurociencia

Ane Escobar Fernández

23/05/2023



El poder de la luz para las tecnologías cuánticas

Gabriel Molina Terriza

23/05/2023

ELHUYAR ZIENTZIA AZOKA

zientzia-azoka.elhuyar.eus

📍 Arenal (Bilbao)

📅 02-04/06/2023

The 11th edition of Elhuyar Zientzia Azoka gathered **200 projects** developed by young students during the course. Since 2019, CFM supports this science fair actively contributing in the mentorship and judging the projects in the fair.

The awards consisted of study grants, trips to national and international fairs and stays in research companies and research centers such as the CFM.

In November CFM hosted the visit of the winners from Lasalle Beasain Ikastola.



"INSPIRA LIVES" IN EUREKA! ZIENTZIA MUSEOA

zientzia-azoka.elhuyar.eus

📍 *Eureka! Zientzia Museoa*, Donostia / San Sebastián

📅 23/10/2023

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 2023, the following researchers from CFM joined this activity, attended by 370 students and 50 professionals:

- Ivan Sasselli (Oral)
- Jorge Humberto Melillo (Poster)
- Paula Angulo Portugal (Poster)



"QUÉ SABEMOS DE..." TALK SERIES

cfm.ehu.es/outreach/quesabemosde

📍 Kutxakultur plaza at Tabakalera, Donostia / San Sebastián

For the seventh consecutive year, the CFM, in collaboration with Kutxa Fundazioa, presents the series *Qué sabemos de...* in Donostia / San Sebastián. This peculiar series of talks, promoted by the Consejo Superior de Investigaciones Científicas (CSIC), is driven by humanity's innate curiosity and features professionals from the realms of science and science communication.

This edition included 3 appointments with cutting-edge science that is shaping the present to transform the future. In addition, in 2023 as a novelty, the talks were accompanied by a dialogue between peers so that we met firsthand not only the science, but the people who carry it out.



Available at
[CFM's YouTube channel](#) or
scanning this
code

Las galaxias antes de que fuesen galaxias

📅 7/11/2023

Speaker: Almudena Alonso Herrero (Centro de Astrobiología en Madrid)

Interviewer: Silvia Bonoli (DIPC)

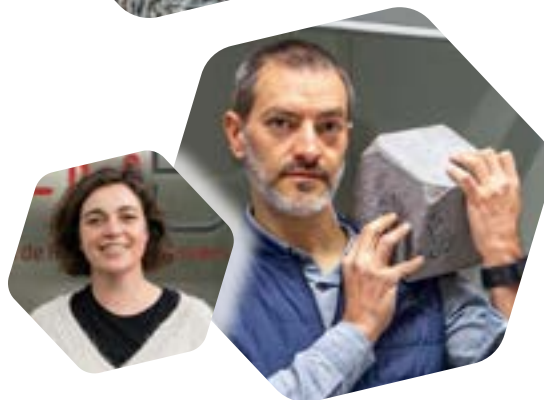


El hormigón verde: Cementando un futuro sostenible

📅 21/11/2023

Speaker: Jorge Sánchez Dolado (CFM)

Interviewer: Idoia Mugica Mendiola (CFM)



Hidrogeno renovable, ¿realidad o reto?

📅 19/12/2023

Speaker: Antonio Chica Lara (Instituto de Tecnología Química)

Interviewer: Sara Barja Martínez (CFM, UPV/EHU)



SCIENCE WEEK 2022 (UPV/EHU)

📍 Tabakalera, Donostia / San Sebastián

📅 9-11/11/2023

STAND "EXPLORING THE WORLD OF MATERIALS"

In this stand DIPC, CIC nanoGUNE, CFM and POLYMAT join forces with a common goal: to bring the science that governs the nature of materials to all audiences. Knowing the properties of matter, studying its physics from an experimental and theoretical point of view, and moving at the nanoscale is essential for the development of new smart materials with multiple applications.

A series of demonstrations and experiments that serve to illustrate the scientific universe behind these "new" materials were presented.

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.

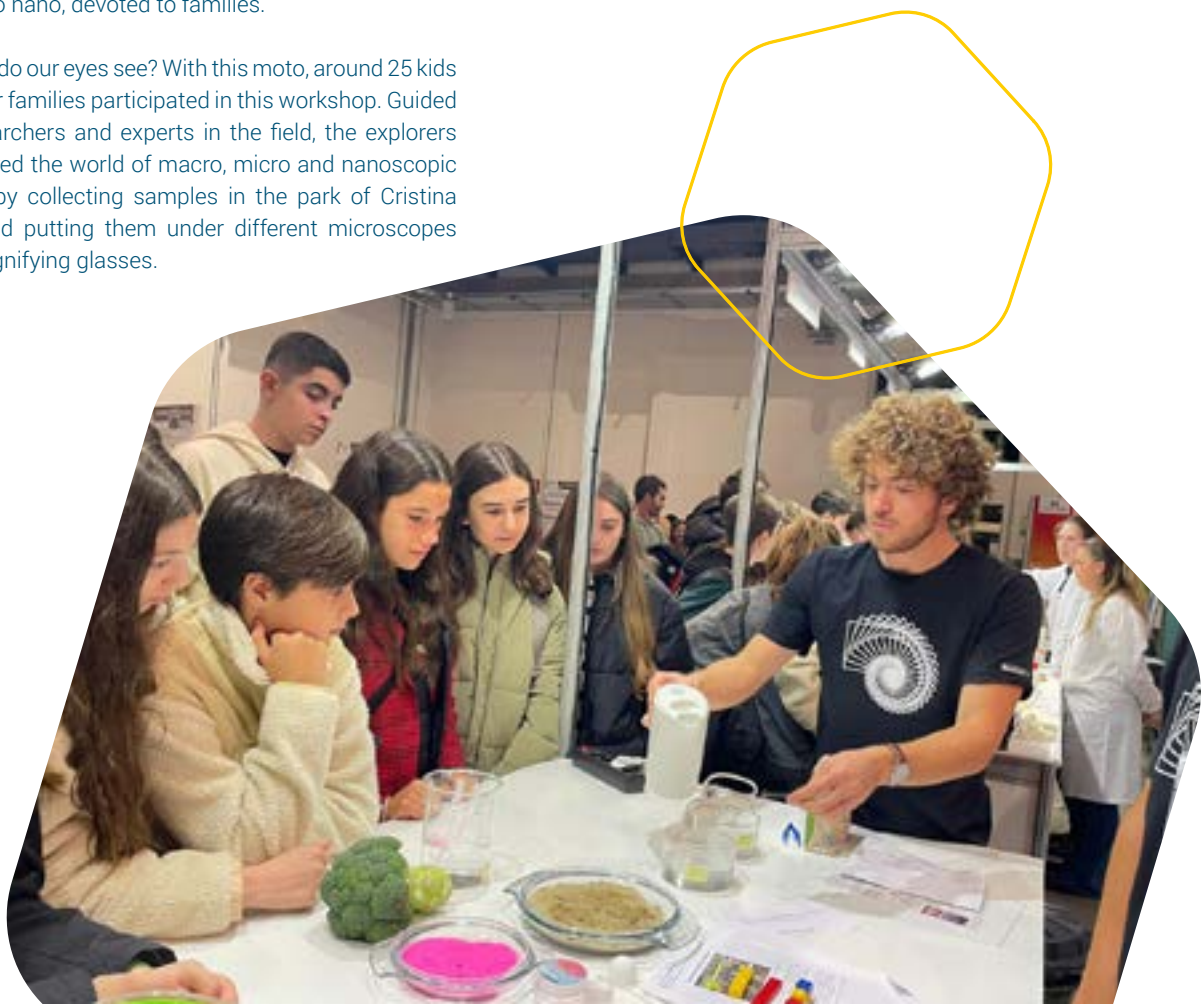
In 2023, CFM outreach manager Idoia Mugica Mendiola participated with the following talk:

Dancing with the microwaves

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 moto, 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.



CINEMA AND SCIENCE

Cycle organized by DIPC and Filmoteka Vasca. CFM researchers participated in the presentation and discussion on the following movies:

Der name der rose

Ricardo Díez Muiño

12/01/2023

Artium Museum (Vitoria)

Pedro Miguel Etxenike Landibar

13/01/2023

Tabakalera (Donostia)

14/01/2023

Bizkaia Aretoa (Bilbao)

17/01/2023

Golem Baiona (Pamplona)

Madame Curie

Nerea Zabala Unzalu

09/02/2023

Artium Museum (Vitoria)

11/02/2023

Bizkaia Aretoa (Bilbao)

23/02/2023

Bizkaia Aretoa (Bilbao)

OTHER OUTREACH TALKS

Ane Escobar Fernández

El oro y las neurotecnologías

18/04/2023

Ciclo Neurotecnologías (DIPC)

San Telmo Museoa, Donostia / San Sebastián

Sara Barja Martínez

Vamos a mover átomos

15/09/2023

Naukas

Bilbao

Ion Errea Lope

Supereroankortasuna, markak hausten!

09/01/2023

Goienagusi

Kulturate, Arrasate

ACTIVITY IN MASS MEDIA

Press articles

47

Online press

132

Radio

50

TV

13

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, collaborated with "Goiz Kronika" radio show running the section "[Zientzia Gosaria](#)" (science breakfast) that is now available as a podcast.



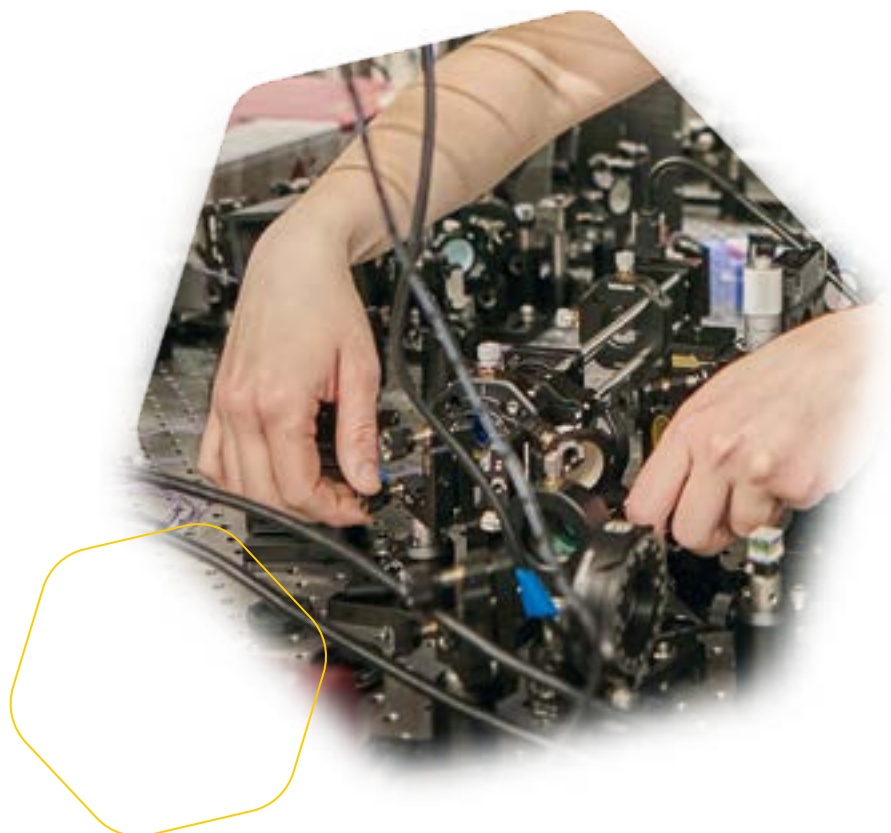
@CFMDONOSTIA

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 2024, CFM had more than **1600 followers in Twitter**, **550 in Instagram**, and **1000 in LinkedIn**. CFM's YouTube channel already contains 48 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

Over the years, the CFM has managed to consolidate a network of active collaboration in the area of scientific dissemination that includes more than 30 science and technology agents in the Basque Country. Thanks to all our allies, it is a pleasure to work side by side to ensure that science reaches all citizens.



GENDER EQUALITY & DIVERSITY



FINAL YEAR OF THE IMPLEMENTATION OF THE GENDER EQUALITY PLAN

"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"

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 about to finish its implementation. Any worker can reach the gender equality committee at any time, in person or at genderequality.cfm@ehu.eus

According to the Gender Equality Plan, there were **31 actions** foreseen for this academic year. The overall implementation of CFM's 1st GEP shows that so far 86% of the actions have been implemented. During 2024 an exhaustive evaluation will take place, which will include a critical overview of the objectives achieved and those on track.



[Read here the full implementation report](#) by scanning this code or visit the [Gender Equality section at CFM's website](#) for related content.

RELEVANT INSTITUTIONAL NEWS

The CFM represents Emakumeak Zientzian in the Equality Council of the Donostia-San Sebastian City Council, which brings together the most relevant feminist associations of the city.

It is also a member of the recently created SCIENCE, TECHNOLOGY AND INNOVATION TECHNICAL GROUP of Emakunde where equality will be addressed specifically in our area of knowledge at the level of the Basque Country.

PREVENTION AND ATTENTION ON HARASSMENT AT CFM

Any issue regarding harassment at CFM can be shared by email harassment.cfm@ehu.eus or talking directly with the personal counselors:

Gabriel Molina Terriza and/or Idoia Mugica Mendiola.

Privacy and anonymity will be guaranteed throughout the process

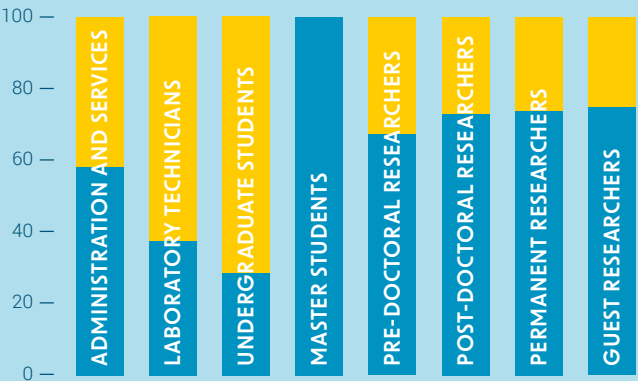
DIAGNOSIS 2023

CFM is committed to run an analysis of the internal situation yearly, publishing the compilation of its own indicators on gender balance. Data of 2023 is presented in the following table and figures:

	♀	♂	
ADMINISTRATION AND SERVICES	10	14	24
LABORATORY TECHNICIANS	5	3	8
UNDERGRADUATE STUDENTS	5	2	7
MASTER STUDENTS	0	4	4
PRE-DOCTORAL RESEARCHERS	27	56	83
POST-DOCTORAL RESEARCHERS	21	57	78
PERMANENT RESEARCHERS	13	37	50
GUEST RESEARCHERS	9	27	36
OTHER GUESTS	1	0	1
	91	200	291

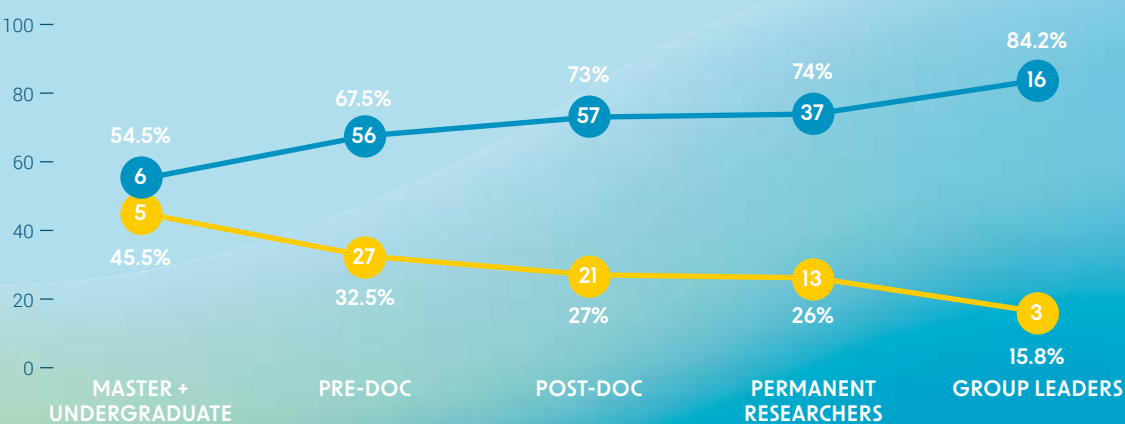
CFM is a highly masculinized workforce (70% men and 30% women at the moment), presenting vertical segregation, with women lacking at top management positions.

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

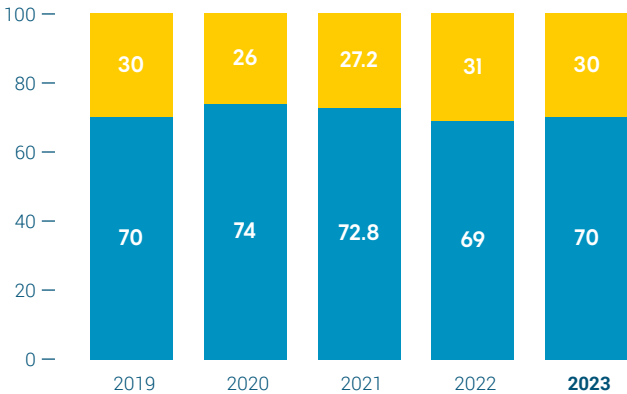


According to this data, the disproportion in the distribution of women/men in the center starts already at the earliest stage of the scientific career. Currently, only 32% of the pre-doctoral researchers at CFM are women. The gender imbalance is accentuated as the responsibility for the job and level 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



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



AWARENESS



EMAKUMEAK ZIENTZIAN

Since its first edition in 2017, “Emakumeak Zientzian” has grown to be a consolidated, award winning, and participation record-breaking consortium, standing out in the set of actions devoted to raising awareness about gender issues at STEM among the society. Nevertheless, it has also been key to build a much-needed network of institutions committed to work together to break the gender divide in the scientific and technological field. **Emakumeak zientzian** has been further described in depth in section *Science and Society* of this report and constitutes the main achievement regarding social awareness on gender issues.

ZERO TOLERANCE

The aim of the plan also includes carrying out activities to raise awareness about gender issues specifically among CFM’s staff. In this regard, among other actions, in 2023 the Gender Equality committee decided to launch the “CFM’s good practice guideline” devoted to CFM’s community, that is available at CFM’s website.

AT CFM WE EXPECT YOU TO

- RESPECT**
Be respectful, empathetic and professional to others. Treat everyone at CFM with respect and dignity regardless of their position and role in the institution. Contribute to a healthy and safe environment at the center.
- DO NOT TOLERATE DISCRIMINATION**
Do not tolerate any form of discrimination at CFM. Contribute to stop any form of abuse, harassment or discrimination you become aware of. If you are aware of such a situation, contact the personnel coordinators at humanresources@cfm.es, your grievance will be guaranteed throughout the process.
- AIRSPACE & HEALTHY WORKING SCHEDULE**
Create a healthy working schedule at CFM. Workday working hours that allow personnel and professional balance. Collective activities will be scheduled in compulsory hours (8:00-18:00) to maximize participation.
- MAKE WOMEN VISIBLE AT THE SCIENTIFIC LEVEL**
For example, encourage all women researchers to write their full names in posters, articles, talks, or any other communication support.
- BE CAREFUL WITH YOUR BIASES**
Pay attention to your unconscious biases in personnel selection and promotion processes. You can check this presentation for further guidance.
- INCLUDE & ZERO TOLERANCE POLICY AT SCIENTIFIC EVENTS**
If you organize a seminar, a workshop, or a congress, state the zero tolerance towards any form of abuse. Announcements of discrimination by adding the following paragraph in the event's web page similar by reading it at the opening:
The organizing committee of 2023 congress for... will guarantee the maximum form of inclusivity, respect and non-discrimination in terms of gender, ethnicity, nationality or other aspects, avoiding harassment or any other type of abuse. We will ensure a safe and healthy work environment for all people.
- GIVE & TRY TO THE INCLUSIVE USE OF LANGUAGE**
Use inclusive language in written and oral expressions, especially when communicating on behalf of CFM. See the document for the inclusive communication at CFM (Appendix).
- PROMOTE DIVERSITY**
Help to improve the visibility of women, ethnic minorities, LGBTQ+ people and other underrepresented collective in science. You can actively join the Emakumeak Zientzian project and the table to be filled collecting contacting the project manager (humanresources@cfm.es).
- THE GENDER EQUALITY COMMITTEE**
genderequality@cfm.es

ANALYSIS OF THE WORK-LIFE BALANCE SURVEY

- Mainly women have difficulties to reconcile their current position with their caring responsibilities.
- Men and women agree on the fact that itinerancy has an impact in their work-life balance, to the extent that (especially women) tend to avoid travelling, attending conferences... due to the rearrangement and the lack of support it entails.
- In general, it seems that both men and women are satisfied with their work/life balance, and caring responsibilities have a positive impact on their responses.

The conference brought together **more than 150 people** around a comprehensive program that included **presentations by experts in the field**, such as Hélène Molinier (Senior Advisor on Digital Cooperation for Gender Equality and thematic responsible for the Action Coalition on Innovation and Technology at UN Women) or Silvia Rueda (Director of the Women and Science Unit of the Ministry of Science and Innovation).



RECRUITMENT PROCESSES

It is essential to address the potential biases that each person may hold regarding this issue to minimize their impact. This issue was confronted with a **specific training on gender biases** devoted to decision making bodies, first organized in 2022, and later compiled in a summary, which is available at CFM's website.

Gipuzkoa Coopera explores the possibility of working together with researchers from countries with less presence in the international scientific community, while involving Gipuzkoa society in the responsibility of collaborating with these countries, promoting scientific activity as an engine of change and progress in any society. With this program CFM also wants to establish its commitment to other social aspects, actively contributing to promoting the development of science in countries with fewer resources.

CFM has been part of the program since its very beginning and over the last six years this has materialized in five collaborations with the foundation **Women for Africa**, through the programs *Ellas Investigan* devoted to senior researchers.



In 2023, CFM welcomed the senior researcher Florette Corinne Fobasso Mbognou (Cameroon) in the Quantum Theory of Materials group to work with Ion Errea.



Florette Corinne Fobasso Mbognou

In addition, CFM on its own initiative, and in conjunction with the DIPC, collaborates in the Learn Africa program, also promoted by the Women for Africa Foundation, aimed at promoting knowledge transfer, exchange and training of African undergraduate and postgraduate students through scholarships. CFM and DIPC provide scholarships to African students to study the UPV/EHU's Master's Degree in Nanoscience taught at CFM. In 2023, CFM and DIPC jointly covered the tuition, travel and monthly living and accommodation expenses of Aja Chioma Ibiam (Nigeria).

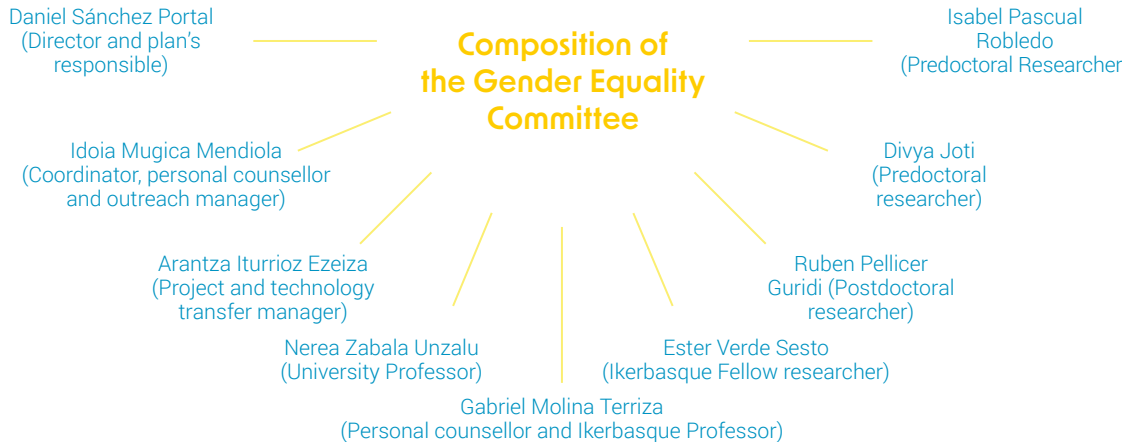


Aja Chioma Ibiam

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 has remained active in the implementation phase and is fully immersed in the design of the II Gender Equality Plan of CFM. Since 2021, Elhuyar, which is approved by *Emakunde* (the Basque Institute for Women) to give technical Gender Equality support to institutions, has provided technical advice and supporting CFM in this major task, and will continue to do so in 2024.



MILESTONES



AWARDS

JAVIER AIZPURUA IRIAZABAL EUSKADI RESEARCH AWARD 2022

The Euskadi Research Award 2022 went to Professor Javier Aizpurua Iriazabal, Research Professor at the CFM and the Donostia International Physics Center (DIPC), and leader of the Nanophotonics Theory group.

In addition to the excellent scientific work of Professor Aizpurua, the jury highlighted his excellent research career and the creation and leadership of a prestigious research group that has become an international reference for its exceptional contributions in the field of quantum phenomena in nanophotonics.



RECOGNITION FOR RESEARCHER SARA BARJA

The Department of Education and Ikerbasque selected the three researchers to be recognized this year, in each of the three levels at which they are awarded. Sara Barja, Ikerbasque Research Associate of the UPV/EHU at the CFM, received recognition at the Starting level. The Committee highlights the unique contributions she has made in her field of research and her recent achievements as a young researcher in a very novel topic, having obtained the ERC Starting Grant that aims to develop new, more efficient and economical catalysts to produce green hydrogen, exploring electrolysis from seawater.



ANGEL RUBIO SECADE NATIONAL RESEARCH AWARD 2023

The National Research Awards, which are Spain's most important recognition in the field of scientific research, honours those researchers who stand out for their careers and international relevance in their respective areas of research. In 2023, the award in the area of Physical, Materials and Earth Sciences went to the physicist Ángel Rubio Secade, from the Max Planck Gesellschaft Institute in Hamburg (Germany) and the CFM. The jury highlighted his extraordinary career and scientific excellence, where his work in computational solid state physics, predicting new properties of materials at the nanoscale and, more recently, new non-equilibrium phases of matter, stand out.



JOSÉ A. POMPOSO ANDREW KELLER AWARD 2022

José A. Pomposo was selected as the winner of the ANDREW KELLER AWARD 2022 for the work "Stars, combs, and bottlebrushes of elastic single-chain nanoparticles".

This award recognizes the best paper published in POLYMER (Elsevier) in 2022 by a European corresponding author. The award ceremony was at the "Frontiers in polymer science" Conference held in Göteborg, Sweden, between May 29 and June 1, 2023.



PABLO GILA HERRANZ WINS THE 2ND PRIZE OF THE MONDRAGON UNIVERSITY AWARDS FOR HIS MASTER THESIS

The MONDRAGON Corporation launched the second edition of the TFG-TFM MONDRAGON Sariaik 2023 Awards. CFM predoctoral researcher Pablo Gila Herranz won the 2nd prize in the Fagor Taldea category for energy-climate transformation for his master thesis work developed in the framework of the Nanoscience master of UPV/EHU, under the supervision of Ikerbasque Professor Felix Fernández Alonso and Kacper Druzicki, from the Quantum Beams and Sustainable Materials group of CFM.



SET UP OF THE NEW MATERIAL FOR QUANTUM TECHNOLOGIES LAB

The first dilution refrigerator in the Basque Country was installed in June 2023 in the CFM. It is the key tool around which the activities of the **new Material for Quantum Technologies group**, led by Dr. Celia Rogero Blanco, Prof. Sebastian Bergeret Sbarbaro, Dr. Max Ilyn, and Dr. Sara Catalano, are organized.

The apparatus is an Oxford Proteox MX 500 and it is installed in the SSA-003 laboratory. With a base temperature of 7 mK and uniaxial magnetic fields of up to 7 T, **this fridge allows for experimental investigation of quantum phenomena in superconductors or in the new topological phases of semiconductors**. Custom copper cold finger and printed circuit board sample holders were designed and fabricated to handle the samples for the DC transport measurements. Cryogenic filters and a modern nano Volt/Ampere meters complement the setup electronics reaching the sensitivity level suitable for characterization of superconducting and semiconducting qubits. The refrigerator is now fully operational. Test measurements were performed on the tunneling and Josephson junctions made in the group of Materials for Quantum Technologies (CFM) and in the Ta nanowires provided by Nanodevices group (NanoGune).

HIGHLIGHTED PAPER FROM THE QUANTUM TECHNOLOGIES LAB

Superconductor-ferromagnet hybrids for non-reciprocal electronics and detectors

Zhuoran Geng, Alberto Hijano, Stefan Ilic, Maxim Ilyn, Ilari J. Maasilta, Alessandro Monfardini, Maria Spies, Elia Strambini, Pauli Virtanen, Martino Calvo, Carmen González-Orellána, Ari P. Helenius, Sara Khorshidian, Clodoaldo I. L. de Araujo, Florence Levy-Bertrand, Celia Rogero, F. Giazotto, F. Sebastián Bergeret, and Tero T. Heikkilä

Superconductor Science and Technology 36, 123001 (2023); Topical Review

In this work, the members of the Nanophysics group and the Mesoscopic physics group together with co-authors review the use of hybrid thin films composed of superconductors and ferromagnets for creating non-reciprocal electronic components and self-biased detectors of electromagnetic radiation.

Major part of this review paper is devoted to explore the applications of S/FI structures in radiation detection. In particular, it is described how an SFTED can be used as a microcalorimeter for X-ray and THz detection. The pronounced thermoelectric effect observed in the devices fabricated in the Laboratory of Materials for Quantum Technologies in collaboration with other members of consortium converts the absorbed energy into an electrical signal without requiring bias power, fundamentally reducing the heat dissipation and wiring complexity of the detector.

Theoretical studies indicate that a superconductor ferromagnet thermoelectric detector (SFTED) has the potential to be a swift cryogenic microcalorimeter. Its energy resolution could rival state-of-the-art ultrasensitive detectors, such as the transition-edge sensor (TES), kinetic inductance detector (KID), and the superconducting tunnel junction (STJ).



Figure 1: Schematic of a (a) superconductor-ferromagnetic thermoelectric detector (SFTED). (b) and (c) are the thermal model and the electrical circuit of the SFTED

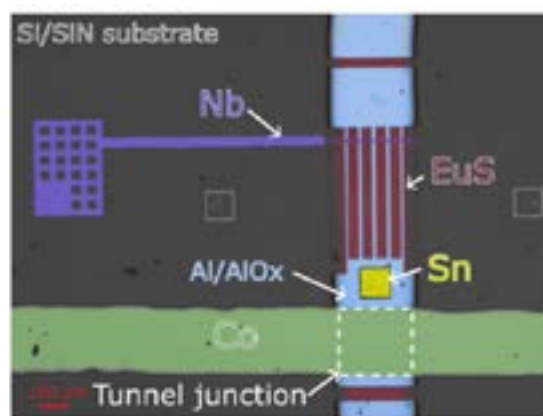


Figure 2: Fake-color optical micrograph of a SFTED calorimeter, in which the material compositions are illustrated with different colors. A superconductor-ferromagnet hetero-junction area is marked with the white dashed line, consisting of layers of Si/SiN/EuS/Al/AlOx/Co from the bottom to the top. A Sn absorber is placed to the side of the junction, contacting directly the Al lead with AlOx layer removed via chemical etching.

**Thanks to
all the CFM
Community**



cfm.ehu.es

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

Report Coordination: Idoia Mugica Mendiola

Edition and corrections: Ioritz Paulis Garmendia
and Idoia Mugica Mendiola

Design: batuta.eus

cfm.ehu.es

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