CFM

Materialen Fisika Zentroa
Centro de Física de Materiales
Materials Physics Center

ACTIVITY REPORT

2022

CSIC
Consejo Superior de Investigaciones Científicas

eman ta zabal zazu
Universidad del País Vasco
Euskal Herriko Unibertsitatea

MPC-BERC
Materials Physics Center
Basque Excellence Research Centre

SUMMARY

FOREWORD

Daniel Sánchez Portal, Director

Year 2022 was the year of the final recovery after the great disruption created by the covid-19 pandemic. Finally, we were able to have normal face-to-face interactions at workshops and conferences. We could welcome again collaborators and friends visiting CFM facilities, organize seminars and travel abroad. We are back to normal and this was highly celebrated by CFM's community. However, the exceptional situation that we went through also brought some positive changes that surely will stay with us. For example, we have realized that teleworking is a good tool that can be used to facilitate conciliation, and that online meetings are a great tool to maintain contact with colleagues and collaborators avoiding travels that were many times unnecessary.

As can be seen in the report, once again 2022 was a good year for science at CFM. We have again produced over 200 publications, including some in the most prestigious journals in our fields of specialization. It has also been an excellent year for fundraising. In total there are 89 projects underway, with close to 7 M€ raised by CFM researchers in 2022 alone, and total rises above 8.3 M€ if we include the MPC-BERC grant from the Basque Government. In addition, 9 doctoral theses have been defended with CFM supervisors. We also keep increasing our technology transfer activity, favoring the creation of collaborations with private companies interested in our research and characterization capabilities. Finally, our commitment to outreach activities has been reflected in the organization of many activities, talks, and our participation in the "Science Week", "Emakumeak Zientzian" and other science popularization festivals.

Especially important during 2022 was the support obtained from the Basque Government through CFM's participation in the IKUR Strategy. In addition to hiring a considerable number of pre- and post-doctoral researchers, the funding obtained through the IKUR Strategy program has made it possible to renew existing and purchase new scientific equipment at CFM and, in particular, to start up a new laboratory for "Materials for Quantum Technologies" with the purchase of a dilution refrigerator capable of going down to millikelvin temperatures. Another milestone related to cryogenics at CFM has been the completion of the construction of a Helium recovery and liquefaction plant. This was possible thanks to the funding coming mainly from the Spanish Research Agency and CSIC. We expect this new facility to be an important boost for CFM's low-temperature scanning tunneling microscopy activity.

Besides the several successes already mentioned above, during 2022 we had other reasons to celebrate.

Iñaki Juaristi Oliden, Vicedirector

At the beginning of 2022 we learned that an ERC Starting Grant was awarded to the project "Controlling Oxygen Selectivity at the Atomic Scale (COSAS)" by our colleague Dr. Sara Barja. We are looking forward to the start of this project in the coming months. The budget of the project is over 2.3 M€, which are not included in the amounts reported above (it will be account for in 2023). Another reason for celebration was the selection of the proposal "Surface Structure and Spectroscopy at 1 bar (3Sbar)" for a new beam line at ALBA synchrotron with an expected cost of 9 M€. This proposal was led by Prof. J. Enrique Ortega, head of the NanoPhysics lab at CFM, and colleagues from ICMAB-CSIC and ALBA, and is expected to provide unprecedented insights on the understanding of fundamental catalytic processes. Finally, the CFM's commitment to promoting the role and visibility of women in science, as well as, its efforts in science dissemination activities was recognized during 2022: "Emakumeak Zientzian (Women in Science)" received the first STEAM Euskadi Prize, awarded by the Basque Government, and the Special Mention Award for Gender Perspective in the category of Most Innovative Initiative in STEAM Education. "Emakumeak Zientzian" was initiated by CICnanoGUNE in 2017 and is currently supported by a large network of research centers in Euskadi. CFM has participated in the event since its second edition in 2018, being one of the coordinators of the network.

The happiest moments of the year came, however, from the miraculously fast recovery of our colleague Prof. Fernando Álvarez González from the extremely serious accident he suffered. We also look forward for the reincorporation during the next weeks of Prof. J. Enrique Ortega after the serious illness that kept him away from the laboratory for more than a year. Dear friends, we are very happy to have you back at CFM.

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

Thank you all for your commitment and support.

Daniel Sánchez Portal
Iñaki Juaristi Oliden

GOVERNANCE

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

DIRECTION BOARD

Director: **Daniel Sánchez Portal**
Vice director: **Iñaki Juaristi Oliden**
Secretary: **Amaia González Azpeitia**

SCIENTIFIC BOARD

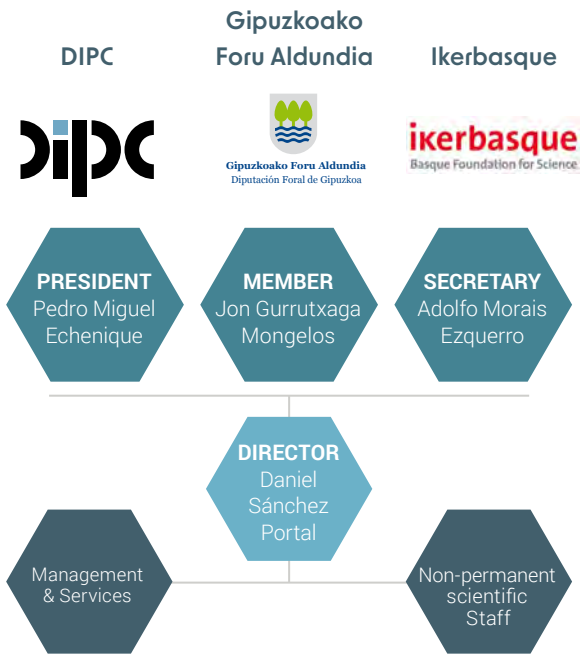
All scientific permanent staff of CFM participates in the Scientific Board. The board is thus composed of UPV/EHU staff, CSIC staff, as well as Ikerbasque staff.

CFM

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

Researchers in Action

264

19

Research Groups

TRAINING

9

PhD Theses defended

15

Master Theses Defended

12

Undergraduate Students

RESEARCH OUTPUT

ISI Publications

207

Q1 Publications

WOS: **56%**

SCOPUS: **84%**

D1 Publications

WOS: **24%**

SCOPUS: **39%**

Citations

14 620

H Index

150

International Collaborations

80%

52%

of the Research Community is international

Researchers from

39

countries

ACTIVITIES AND EVENTS

Conferences, Workshops, Courses, and Seminars

25

Science and Society

+70 Activities

+40 Volunteers

+10 000 Atendees

PROJECTS AND FUNDING

Ongoing Projects

89

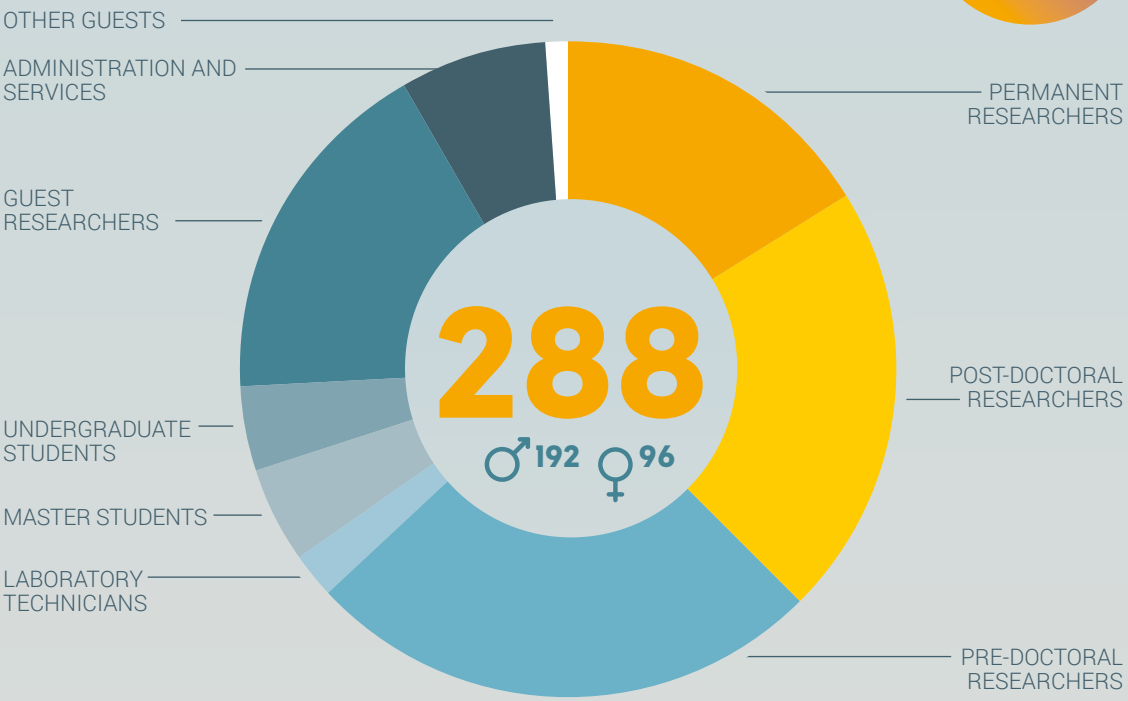
Funding

8 325 983.39 €

PEOPLE

ALL THE CFM COMMUNITY

Full Gender diagnosis in GENDER EQUALITY & DIVERSITY section of this report



CFM Staff

214

Researchers in Action

264 [3]

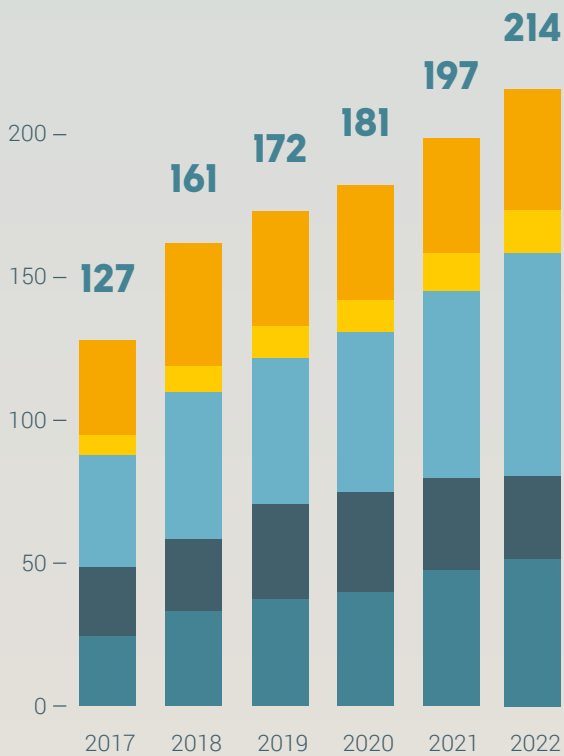
Permanent Researchers	47
Post-doctoral Researchers	61
Pre-doctoral Researchers	74
Laboratory Technicians	6
Master students [1]	14
Undergraduate students [2]	12
Guest Researchers	50
Administration and Services	21
Other guests	3
Total	**288**

[1] Four of those receive scholarships during their stay at CFM and are considered staff
[2] One of those receive scholarships during their stay at CFM and are considered staff
[3] Including Guest researchers, undergraduate and master students

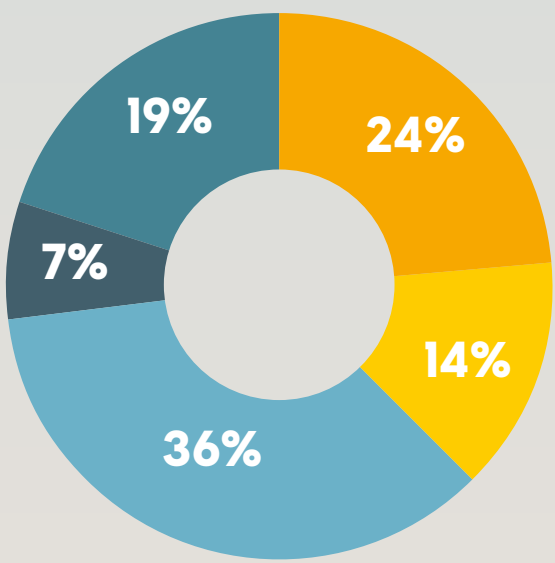
DISTRIBUTION OF CFM STAFF according to the origin of the financial support

	2017	2018	2019	2020	2021	**2022**
CSIC	24	33	37	40	47	**51**
UPV/EHU	24	25	33	34	32	**29**
MPC-BERC	39	51	51	56	65	**77**
IKERBASQUE	7	9	11	11	13	**15**
COLLABORATORS	33	43	40	40	40	**42**
Total	127	161	172	181	197	**214**

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 2022



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
Arantza Iturrioz Ezeiza, Project and Technology Transfer Manager, MPC
Arkaitz Nagore Ibero, Public Procurement Manager, MPC
Elixabet Sarasketa Zabala, Project and Technology Transfer Manager, MPC
Idoia Mugica Mendiola, Outreach Manager, MPC
Laura Alfonso Zarra, Administrative, MPC
María Formoso Ferreiro, Administrative, MPC
María José Sánchez Álvarez, Executive Secretary, UPV - EHU
Marta López Pérez, Administrative, MPC
Tineke 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, Computer Center Manager, CSIC
Ioritz Paulis Garmendia, IT Systems Technician, MPC
Irene Azáceta Elzaurdi, , Scientific Computing Service, MPC
Mikel Arocena Errazquin, Scientific Computing Service, MPC
Urtzi Oliveras Egaña, IT Systems Internship, MPC

MAINTENANCE

Ekain Ugalde Goldarazena, MPC
Juan Manuel Burgos Jiménez, MPC

LABORATORY TECHNICIANS

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

Chemical Physics of Complex Materials

01 Gas/Solid Interfaces

PERMANENT RESEARCHERS
Iñaki Juaristi Oliden, University Professor, UPV/EHU
Maite Alducin Ochoa, Tenured Scientist, CSIC
Ricardo Díez Muiño, Research Scientist, CSIC

POST-DOCTORAL RESEARCHERS
Alfredo Serrano Jiménez
Alberto Pablo Sánchez Muzas
Raúl Bombín Escudero

PRE-DOCTORAL RESEARCHERS
Auguste Tetenoire
Ivan Zugec

UNDERGRADUATE STUDENT
Iñaki Fernández Tena

GUEST RESEARCHERS
Andrey Postnikov, Scientific Senior
Federico González, PhD Student

02 Quantum Phenomena on Surfaces

PERMANENT RESEARCHER
Nicolás Lorente Palacios, Research Scientist, CSIC

SCIENTIFIC SENIOR
Roberto Robles Rodriguez

IKERBASQUE FELLOW
Deung-Jang Choi, MPC

PRE-DOCTORAL RESEARCHERS
Cristina Mier González
Divya Jyoti
Mireia Tena Zuazolacigorraga

GUEST RESEARCHERS
José Reina Gálvez, Post Doc
Paula Abufager, Scientific Senior
Parmenio Boronat, Master Student
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
Maider Ormaza Saezmiera, Associate Professor, UPV/EHU
Martina Corso, Tenured Scientist, CSIC

RAMON Y CAJAL RESEARCHER

Sara Barja Martínez

POST-DOCTORAL RESEARCHERS

Andrew P. Weber
Jan Patrick Calupitan
Jesús Rubén López-Roso Redondo
John Fredy Vélez Santa
Jose Eduardo Barcelon
Marco Gobbi (Ikerbasque Fellow on leave at CIC nanoGUNE)
Maxim Ilin
Rishav Harsh
Sabine Auras
Yuri Hasegawa

PRE-DOCTORAL RESEARCHERS

Alaa Mohammed Idris Bakhit
Amitayush Jha Thakur
Andrea Aguirre Baños
Carmen González Orellana
David Caldevilla Asenjo
Paula Angulo Portugal
Rodrigo Castrillo Bodero
Sandra Sajan
Samuel Kerschbaumer

GUEST RESEARCHERS

Adelina López Romers, Master Student
Alfonso Yubero Navarro, Master Student
Camilo Arturo Mesa Zamora, Post-Doctoral Researcher
Dominik Bogumil Wrana, Post-Doctoral Researcher
Estephania Lira Salazar, Scientific Senior
Ignacio Piquero Zulaica, Post-Doctoral Researcher
Javier García de Abajo, Scientific Senior
Naia Mondragón Arrese, Master Student
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

POST-DOCTORAL RESEARCHERS

Mikhail Otrokov

PRE-DOCTORAL RESEARCHERS

Joseba Goikoetxea Perez
Malen Etxeberria Etxaniz
Masoud Mansouri
Sophie Espert

GUEST RESEARCHER

María Blanco Rey, Scientific Senior

05 Spectroscopy at Atomic Scale

PERMANENT RESEARCHER

Lucia Vitali, Ikerbasque Professor, UPV/EHU

GUEST RESEARCHER

Xabier Guerrero Ricarte, Master Student

06 Theoretical and Computational Chemistry

PERMANENT RESEARCHER

Pedro Braña Coto, Research Scientist, CSIC

POST-DOCTORAL RESEARCHERS

Giulia Biffi
Stefano Sansotta

GUEST RESEARCHER

Juan Andrés Bort, Scientific Senior
Kathir R. K. , Post-Doctoral Researcher
Luis Antonio Cabral, Post-Doctoral Researcher

Electronic Properties at the Nanoscale

07 Electronic Excitations in Surfaces and Nanostructures

PERMANENT RESEARCHERS

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

POST-DOCTORAL RESEARCHERS

Ilya Nechaev
Rodrigo Humberto Aguilera del Toro

PRE-DOCTORAL RESEARCHERS

Jozef Janovec
Mikel Arruabarrena Larrarte
Raúl Guerrero Avilés

GUEST RESEARCHERS

Diego Edmundo Lauer Zegarra, Pre-doctoral Researcher
Jhon Wilfer González Salazar, Scientific Senior
Karolina Slowik, Scientific Senior
Marta Zuzanna Pelc, Scientific Senior

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
Francesco Belli
Josu Diego López
Martín Gutiérrez Amigo
Oscar Rodríguez Ballesteros

GUEST RESEARCHERS

Jorge Diogo Marques Laranjeira, Pre-doctoral Researcher
Trinidad Novoa Aguirre , Pre-doctoral Researcher

09 Mesoscopic Physics

PERMANENT RESEARCHER
F. Sebastián Bergeret Sbarbaro, Research Scientist, 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
Cheol-Hwan Park DIPC
Óscar Pozo Ocaña

GUEST RESEARCHERS
Mads Kruse, Pre-doctoral Researcher
MooYoung Choi, Scientific senior
Seungju Hong, Pre-doctoral Researcher
Yangjun Lee, Pre-doctoral Researcher

12 Ceramic and Cement-Based Materials

PERMANENT RESEARCHER
Jorge Sánchez-Dolado, Research Scientist, 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

GUEST RESEARCHERS
Mary Bosede Ogundiran, Scientific Senior
Miguel Beruete, 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

GUEST RESEARCHER

Manuel Dos Santos Dias, Scientific Senior

Photonics

14 Theory of Nanophotonics

PERMANENT RESEARCHERS

Javier Aizpurua Iriazabal, Research Professor, CSIC
Nerea Zabala Unzalu, University Professor, UPV/EHU
Rubén Esteban Llorente, Tenured Scientist, CSIC

POST-DOCTORAL RESEARCHERS

Antton Babaze Aizpurua
Mario Zapata Herrera
Roberto Álvarez Boto
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

Cesar Herreño Fierro, Scientific Senior
Emma Furlanetto, Master Student
Fernando Aguilar-Galindo Rodríguez, Scientific Senior
Jinna He, Scientific Senior
Panagiota Elli Stamatopoulou, Pre-doctoral Researcher
Pawel Hawrylak, Scientific Senior

15 Nanomaterials and Spectroscopy

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

POST-DOCTORAL RESEARCHERS
Adam Olejniczak
Ane Escobar Fernández
María Sanromán Iglesias
Victor Krivenkov

PRE-DOCTORAL RESEARCHERS
Alba María Jumbo Nogales
Joscha Kruse
Zuzanna Lawera

UNDERGRADUATE STUDENT
León Begiristain Ribó

GUEST RESEARCHERS
Aimar Marauri Iriberri, Master Student
Elisa Erice Ainciburu, Master Student
Juliette Lacherez, Undergraduate
June Aguirre Tolosa, Master Student
Maciej Baginski, Post-doctoral Researcher
Mikhail Igorevich Vasilevskiy, Scientific Senior

16 Laser Physics 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
Juan José Miguel Varga
Rubén Pellicer Guridi
Sergio Sánchez Martín

PRE-DOCTORAL RESEARCHERS
Iker Gómez Viloria
Isaac Tribaldo Ramírez
Jon Lasa Alonso
María García Alonso
Martin Molezuelas Ferreras
Mikel Elorza Romera
Miriam Martínez Flórez
Shah Jee Rahman

MASTER STUDENT
Joseba Solozabal Aldalur

GUEST RESEARCHERS
Kostiantyn Bliokh, Scientific Senior
Mathis Carpenter, Master Student
Koen Clusters, Undergraduate

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

IKERBASQUE ASSOCIATE

Armando Maestro Martín

IKERBASQUE FELLOWS

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

POST-DOCTORAL RESEARCHERS

Beatriz Robles Hernández
Jorge Humberto Melillo
Mounika Gosika
Nisha Pawar
Soheil Sharifi
Valerio Di Lisio
Soheil Sharifi
Valerio Di Lisio

PRE-DOCTORAL RESEARCHERS

Adil Hamid
Agustín Blazquez Martín
Carlo Andrea Pagnacco
Claudia Borredon
Davide Arena
Eric Gómez Urreizti
Francesco Coin
Javier Martínez Sabando
Jokin Pinacho Olaciregui
Luis Alejandro Miccio Stefancik
Maiara Aime Iriarte Alonso
Mariarita Paciolla
Matteo Sanviti
Numera Shafqat
Thu Phuong Le
Vasiliki-Maria Stavropoulou

GUEST RESEARCHERS

Anabel Lam Barandela, Scientific Senior
Analia Dall´Asen, Scientific Senior
Carlos Andrés Peniche Covas, Scientific Senior
Chizoba May Obele, Post-doctoral Researcher
Chokri Llucia Arza, Undergraduate Student
David Gutiérrez Armayor, Master Student
Elisa Sturabotti, Post-doctoral Researcher
Jorge Manuel Méndez, Scientific Senior
José Vega-Baudrit, Scientific Senior
Katelyn Samantha Randazzo , Pre-doctoral Researcher
Manuel Gómez Menéndez, Master Student
Marta Aldecoa Ortueta, Undergraduate Student
Mikel Iguaran Aguirregomezcorta, Undergraduate Student
Miriam Peña Figueroa, Undergraduate Student
Pablo Ruíz Bozal, Master Student
Santiago Estévez Areco, Post-doctoral Researcher
Silvia Nair, Scientific Senior

19 Quantum Beams and Sustainable Materials

PERMANENT RESEARCHER

Felix Fernández Alonso, Ikerbasque Professor, MPC

POST-DOCTORAL RESEARCHER

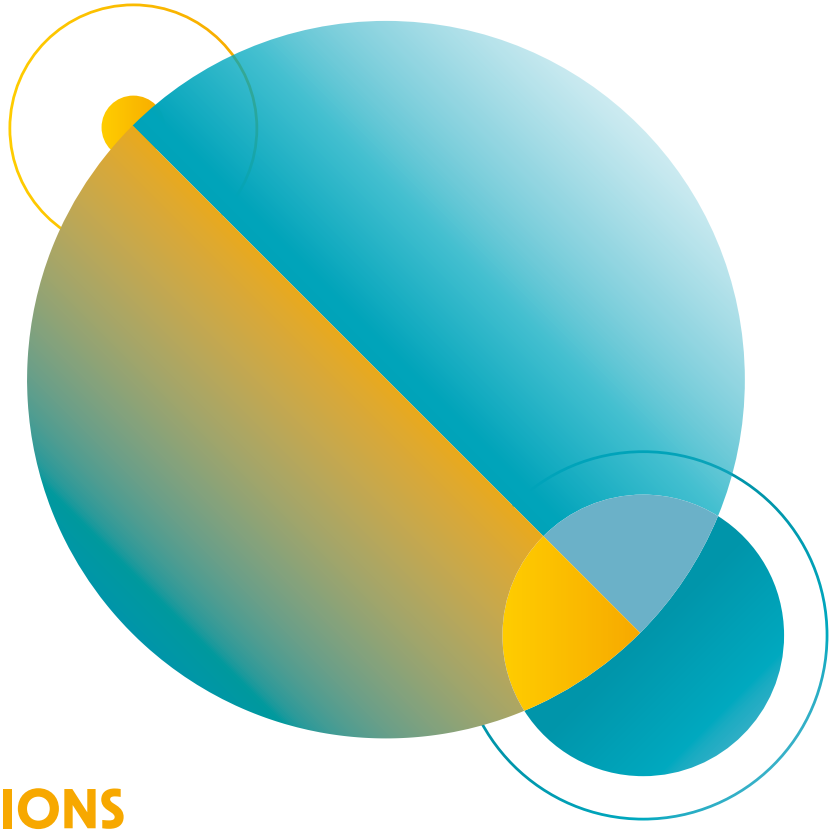
Kacper Druzbicki

PRE-DOCTORAL RESEARCHERS

Balthasar Braunewell
Cristina Maciá Castello
Pelayo Marín Villa

GUEST RESEARCHERS

Oksana Korolyuk, Scientific Senior
Margherita Simoni, Undergraduate Student



OTHER POSITIONS

SCIENTIFIC SENIORS

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

POST-DOCTORAL RESEARCHER

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

PRE-DOCTORAL RESEARCHERS

Alejandro Berdonces Layunta, DIPC (Dimas García de Oteyza's group)
Miguel Ángel Jiménez Herrera, MPC (Dario Bercioux's group)
Pablo Herrero Gómez, DIPC (Celia Rogero's group)
Paul Lukas Dreher, DIPC (Miguel Moreno Ugeda's group)

MASTER STUDENTS

Edurne Sáenz Parraga
Lorea Sánchez Fernández de Larrea
Martin Irizar Landa

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

Group Leader: Ricardo Díez Muiño, Research Scientist CSIC

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

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

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

2

Quantum Phenomena on Surfaces

Group Leader: Nicolás Lorente Palacios, Research Scientist CSIC

The activity of the **Quantum Phenomena on Surfaces** group focuses on the development of computational schemes to unveil the richness of realistic spectral functions, with Dr. Deung-Jang Choi leading the experimental work and Dr. Nicolas Lorente leading the theoretical work. The main research topics in the group are electronic, vibrational and magnetic excitations, particularly of molecular and nanomagnetic systems on solid surfaces, ranging from semiconductors and metals to superconductors.

In recent years, the following objectives have been addressed on these topics: (i) the use of density functional theory to understand the geometrical and electronic structure of different surface systems, and (ii) the development of theories and numerical treatments to understand phenomena revealed by STM.

3

Nanophysics Lab

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

The **NanoPhysics Lab** (NPL) group studies structural, electronic, magnetic and chemical properties of in-situ and ex-situ grown nanostructures in the context of experimental surface science. NPL aims at exploring relevant but yet-widely-unknown phenomena taking place at the surface of solid materials, such as the atomic-level control of on-surface chemical reactions and catalysis, the bottom-up fabrication of 1D or 2D functional materials, and also the growth of novel layered materials with potential application in state-of-the-art technology devices. 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

Group Leader: Daniel Sánchez Portal, Research Professor CSIC

The activity of the **Modelisation and Simulation** group focuses on the theoretical study of the electronic and structural properties of complex materials, clean and decorated surfaces, and nanostructures. It pursues the following objectives: (i) to develop the basic theory and ab-initio simulation tools in order to study the behavior of different nanoelectronic devices, particularly those based on graphene derivatives, (ii) to study the optical properties of complex organic/inorganic interfaces, (iii) to study the magnetic properties of different nanostructures, ranging from one dimensional systems to coordination networks and multilayer heterostructures at surfaces, and (iv) to continue to foster the development of the SIESTA code.

Most of the research activity of this group is performed in close collaboration with other experimental and theoretical groups at CFM, and also with groups from other research centers in the Basque Autonomous Community.

5

Spectroscopy at Atomic Scale

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

The activity of the **Spectroscopy at Atomic Scale** group is devoted to explore the structural and spectroscopic characteristics of materials at the local scale, with the use of Scanning Tunneling Microscopy (STM) techniques. The objectives of this activity focus on: (i) the understanding of different mechanisms that influence the electronic, magnetic and vibrational properties on surfaces, (ii) the study of electron transport and chemical reactivity of surface supported nanostructures, (iii) the investigation of new strategies leading to the formation of covalently bonded conjugated structures with functional groups, and (iv) two dimensional properties emerging in layered materials.

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

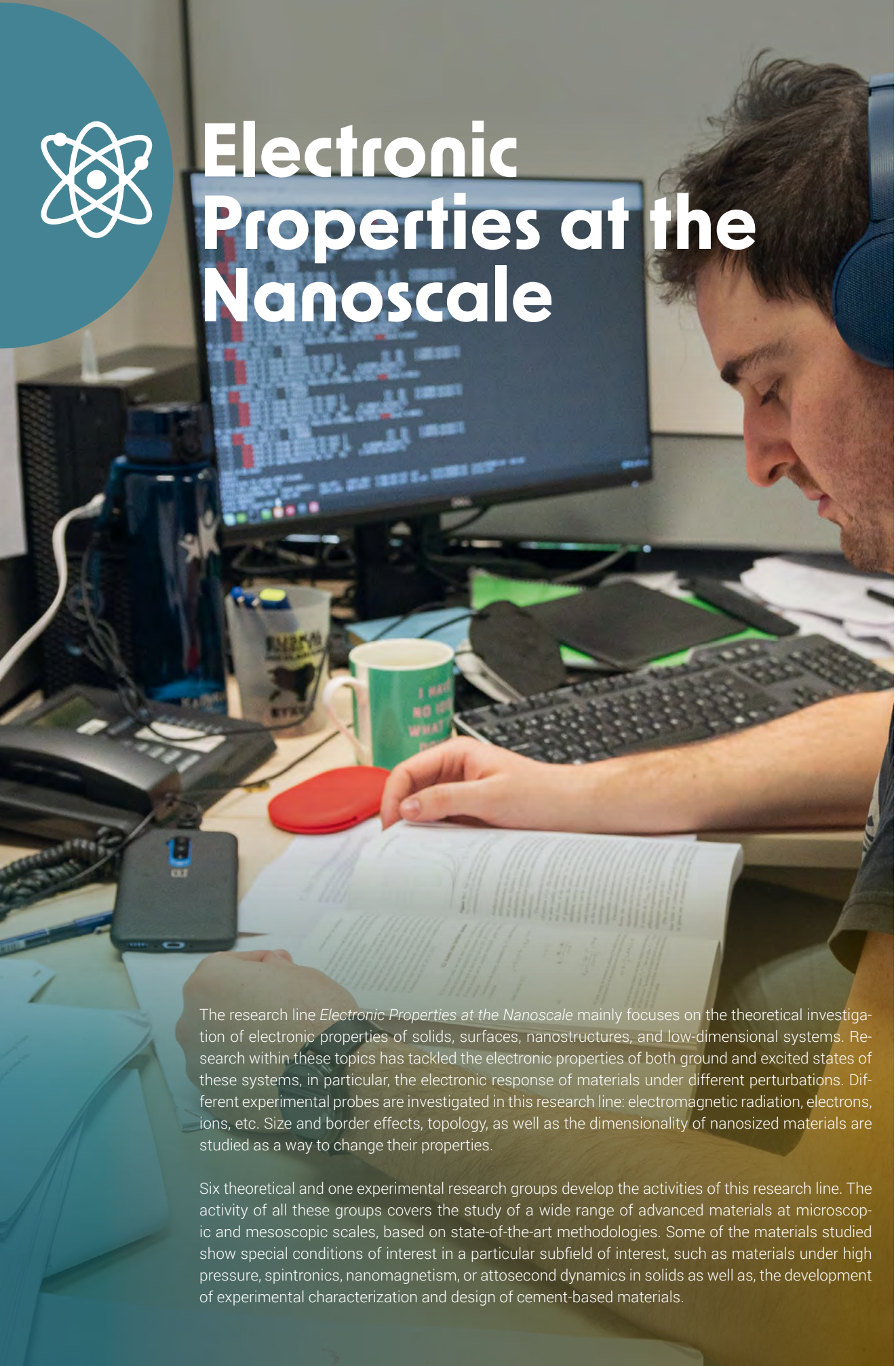
6

Theoretical and Computational Chemistry

Group Leader: Pedro Braña Coto, Research Scientist CSIC

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

Electronic Properties at the Nanoscale



The research line *Electronic Properties at the Nanoscale* mainly focuses on the theoretical investigation of electronic properties of solids, surfaces, nanostructures, and low-dimensional systems. Research within these topics has tackled the electronic properties of both ground and excited states of these systems, in particular, the electronic response of materials under different perturbations. Different experimental probes are investigated in this research line: electromagnetic radiation, electrons, ions, etc. Size and border effects, topology, as well as the dimensionality of nanosized materials are studied as a way to change their properties.

Six theoretical and one experimental research groups develop the activities of this research line. The activity of all these groups covers the study of a wide range of advanced materials at microscopic and mesoscopic scales, based on state-of-the-art methodologies. Some of the materials studied show special conditions of interest in a particular subfield of interest, such as materials under high pressure, spintronics, nanomagnetism, or attosecond dynamics in solids as well as, the development of experimental characterization and design of cement-based materials.

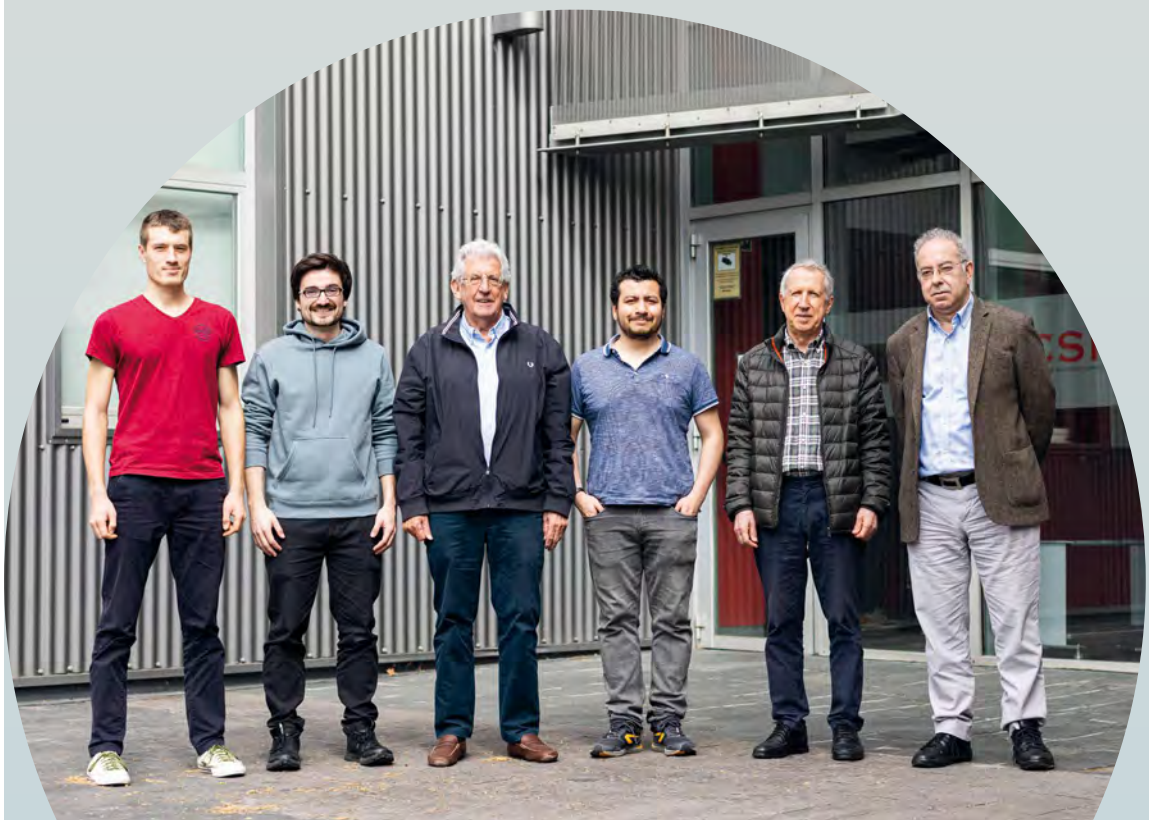
7

Electronic Excitations in Surfaces and Nanostructures

Group Leader: Andrés Ayuela Fernández, Research Scientist CSIC

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

In recent years, electronic and magnetic properties of materials have been investigated by this group using first principles methodologies. Electron dynamics in different systems have been also studied, with particular emphasis on ultrafast processes and size effects. Advanced materials, such as topological insulators and cement-related systems, are current targets of these activities



8

Quantum Theory of Materials

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

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

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

9

Mesoscopic Physics

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

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

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

10

Nano-Bio Spectroscopy

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

The activity of the **Nano-Bio Spectroscopy** group is devoted to the field of theory and modelling of condensed matter electronic and structural properties, with special emphasis in the optical response of nanosystems. A strong program focusing on developing novel theoretical tools and computational codes to investigate the electronic response of solids and nanostructures to external electromagnetic fields has been settled in this group. The main research interests of this activity are as follows: (i) foundations of time-dependent density functional theory for biophysics, (ii) foundations of the many-body theory, (iii) electronic and thermal transport, (iv) theory of open quantum systems, and (v) strong light-matter interactions and optimal control theory.

In recent years, the main research activities on these topics include new developments within the many-body theory and TDDFT, covering ab-initio descriptions of electron excitations, optical spectroscopy, time-resolved spectroscopies, and lifetimes. Novel techniques to calculate total energies have also been developed, assessing exchange correlation (XC) functionals for TDDFT calculations. Improvements on transport theory within the real-time TDDFT formalism have also been achieved. Moreover, the electronic and optical properties of solids, nanostructures (in particular nanotubes, nanowires and semiconducting -clusters-) and biomolecules is also tackled in the group. All these activities have resulted in the establishment of the European Theoretical Spectroscopy Facility (ETSF).

11

Souza Group

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

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

In recent years, the work has involved the development of new theoretical approaches and algorithms, and their application to problems of current interest, including methods to study insulators in finite electric fields, as well as to construct localized Wannier orbitals for metals. Phenomena that arise from the interplay between the collective magnetic order in solids and the spin-orbit interaction inside the constituent atoms have been also successfully addressed.

12

Ceramic and Cement-Based Materials

Group Leader: Jorge Sánchez Dolado, Tenured Scientist, CSIC

The group researches a variety of properties of cement-based and ceramic materials experimentally and theoretically. Combining knowledge from different disciplines, like solid-state physics, soft-matter physics, geochemistry and chemical engineering, the "Ceramic and Cement-based Materials" group focuses on the computational design and synthesis of new ceramic and cement-based materials with lower CO_2 fingerprint.

The initial objectives of the group are: (i) the use of atomistic and colloidal simulations to study the structure and properties of cement-based materials, (ii) the implementation of new technologies in hydrothermal and supercritical fluids (SCF) for the ultra-fast synthesis of ceramic nanoparticles, (iii) the development of new sintering methodologies through the use of autoclaves or microwaves that allow notable energy savings and a drastic reduction of CO_2 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

Group Leader: Julen Ibañez Azpiroz, Ikerbasque Research Associate

The European Research Council (ERC) granted 1.4 million euros to Julen Ibáñez, Ikerbasque researche associate from the UPV/EHU at CFM, in the ERC Starting Grant call for proposals. Thanks to this grant, in 2022 Dr Ibañez was able to start creating his own research team, which will be fully operative in 2023.

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 behavior 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

Group Leader: Javier Aizpurua Iriazabal, Research Professor, CSIC

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

In recent years, the following specific objectives have been addressed by this group: (i) understanding and characterization of the collective excitations of an electron gas in nanostructures, the so-called surface plasmons, in a variety of spectroscopy and microscopy techniques, (ii) study of metallic nanostructures as electromagnetic field enhancers and localizers, (iii) development of protocols and models to better interpret and describe the images obtained by the scattering-type scanning near-field optical microscope, (iv) study and exploitation of the interaction of fast electrons and matter to develop new paradigms of spectroscopy in the nanoscale, (v) description of quantum effects derived from the coherent nature of the electrons that constitute a plasmonic excitation, (vi) study of the magnetic activity of dielectric nanostructures at optical frequencies, (vii) characterization of the dynamics and the coupling of emitters to be used in quantum information technology, and (viii) address non-linearities and collective effects in molecular optomechanics.

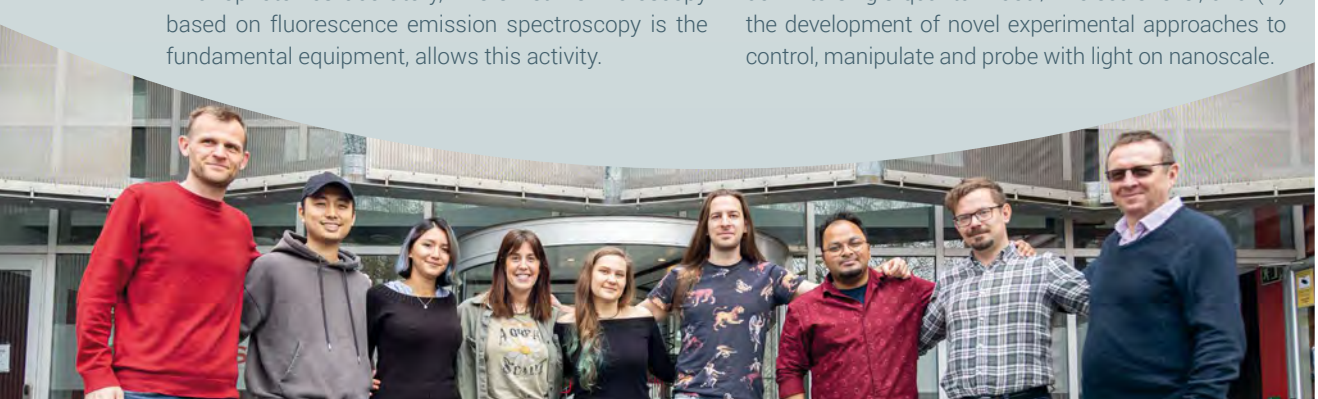
15

Nanomaterials and Spectroscopy

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

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

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



16

Laser Physics and Photonic Materials

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

The activity of the **Laser Physics and Photonic Materials** group concentrates most of the research efforts on the study of 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 vitroceramics for integrated optics applications, (ii) the study of the laser emission processes in dye-doped micro-nano structured hybrid materials for optoelectronic and biomedical applications, (iii) the synthesis and development of new eutectic materials for biomedical applications, (iv) the 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

Gabriel Molina Terriza,
Ikerbasque Professor, MPC

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

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

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

Polymers, Soft Matter & Sustainable Materials P(SM)$_2$

The research line *Polymers and Soft Matter* focuses on the experimental and theoretical study of the structure and dynamics of complex molecular systems with an emphasis on polymers, soft matter and functional materials. The "Quantum Beams and Sustainable Materials" group (19) complements this research line, expanding the field of research and expertise on this area.

18

Polymers & Soft Matter

Juan Colmenero de León,
University Professor, UPV/EHU

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

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

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

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HIGHLIGHT 1 – Gas/Solid Interfaces

Why ultrafast photo-induced CO desorption dominates over oxidation on Ru(0001)

Auguste Tetenoire, Christopher Ehlert, J. Iñaki Juaristi, Peter Saalfrank, and Maite Alducin.

Journal of Physical Chemistry Letters 13, 8516 (2022)

CO oxidation on Ru(0001) is a long-standing example of a reaction that, being thermally forbidden in ultra-high vacuum, can be activated by femtosecond laser pulses. In spite of its relevance, the precise dynamics of the photo-induced oxidation process as well as the reasons behind the dominant role of the competing CO photo-desorption have so far remained unclear.

Irradiation of a metal surface with femtosecond laser pulses generates a transient nonequilibrium distribution of hot electrons that subsequently transfer their energy to the surface phonons and also to the adsorbate degrees of freedom. This strong perturbation can lead to the emergence of completely new phenomena such as the opening of new reaction channels that cannot be accessed by thermal activation.

The oxidation of CO on Ru(0001) is precisely the emblematic example of a reaction that, being thermally forbidden in ultra-high vacuum, can be activated by femtosecond laser pulse irradiation, as was first found experimentally in Bonn et al. Science 285, 1042 (1999). Nonetheless, in spite of its relevance, the precise dynamics of the photo-induced CO oxidation process as well as the reasons behind the surprising dominant role of the competing CO photo-desorption process have remained unclear.

In this work, Tetenoire and co-workers investigate these two reactions with ab initio molecular dynamics with electronic friction that account for the non-equilibrated and highly excited electrons and phonons created by the laser. Their simulations successfully reproduce the

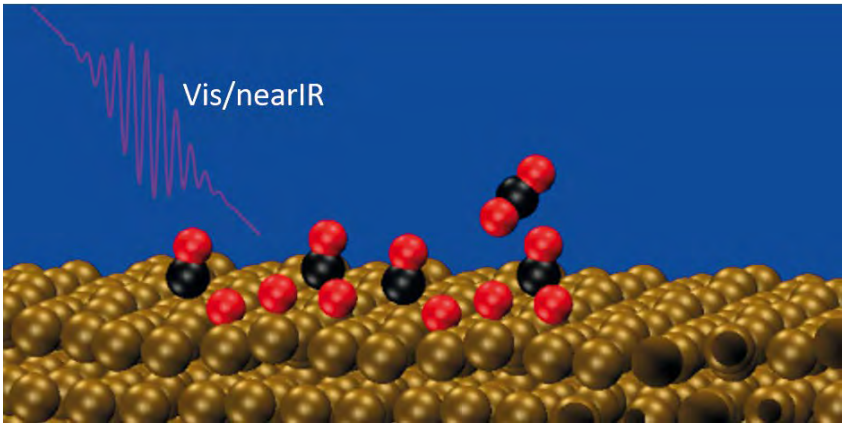


Figure 1: *Art image of the recombinative desorption of CO_2 induced by femtosecond laser pulses*

main features observed in the experiments such as the photo-desorption of CO and CO_2, the large CO desorption to CO oxidation branching ratio, and the changes in the O K-edge X-ray absorption spectra attributed to the initial stage of the CO oxidation process. Importantly, the authors are finally able to monitor step by step how the ultrafast CO desorption and CO oxidation occur in the highly-excited system and explain why CO desorption dominates over the energetically favored oxidation. It is the O adsorbed at the fcc sites that primarily recombines with the adsorbed CO, following basically the intermediate extreme states of the minimum energy oxidation path. The reason behind the unexpected inertness to the otherwise energetically favored oxidation is two-fold: (i) the difficult access to the transition state region, that requires the O atom crossing the bridge site and finding the CO conveniently close and tilted to form the chemisorbed bent CO_2 and (ii) the fact that this access does not guarantee a successful recombination.

In this work, the authors improve over a classical trajectory method by including quantum corrections. The interaction between the molecules and the surface are described by density functional theory. They assign statistical weights to classical paths on the basis of two semiclassical corrections: gaussian binning and the adiabaticity correction.

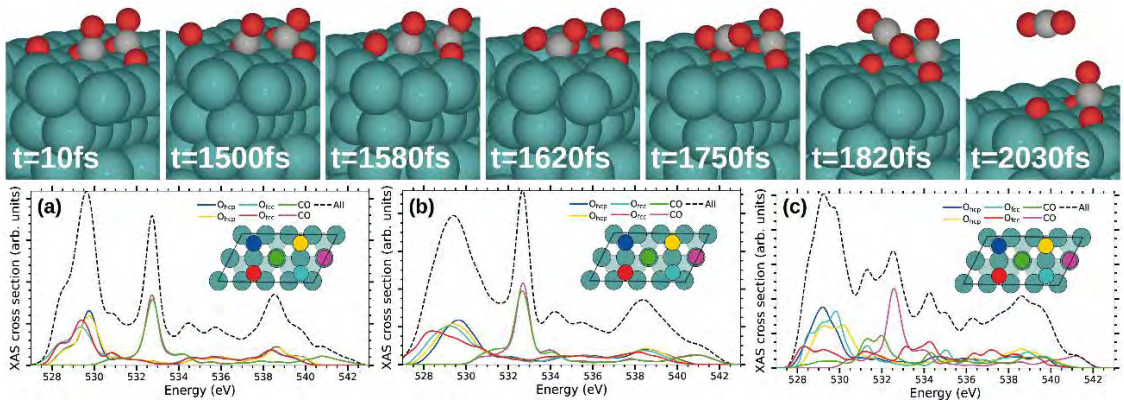


Figure 2: *Top- Snapshots of a representative CO oxidation dynamics obtained in the (Te,Tl)-AIMDEF simulations (blue, red, and gray spheres correspond to Ru, O, and C atoms, respectively). The AIMDEF simulation time is indicated in each panel. Bottom- Time averaged O-K XAS cross section calculated at characteristic time intervals during the oxidative desorption process in the selected trajectory: (a) initial strong excitation of the adsorbates (0-1250 fs), (b) access to the transition state ruling the reaction, in which the recombining Ofcc reaches the bridge site that separates it from the nearest CO (1250-1580 fs), and (c) formation of the chemisorbed bent CO_2 (1600-1630 fs). Each color curve shows the contribution of the corresponding colored O atom depicted in the surface unit cell plotted as an inset. Black dashed curves show the total time-averaged XAS.*

HIGHLIGHT 2 – Quantum Phenomena on Surfaces

Moiré dispersion of edge states in spin chains on superconductors

Cristina Mier, Deung-Jang Choi, and Nicolás Lorente.

Physical Review Research 4, L032010 (2022)

Majorana bound states have been predicted at the edge of spin chains on s-wave superconductors. Recent experiments show zero-energy edge states that could be Majorana bound states but they turn out to depend on the spin chain size, leading to strange energy oscillations with the length of the spin chain. This work shows that they are indeed Majorana bound states that are mixed with other in-gap states due to finite size effects. The behavior of the energy originates in the electronic oscillations as contain in the Fermi wave length and in the spin chain periodicity, leading to a moiré pattern that translates into energy oscillations of the lower-energy edge states.

Recent experimental work by Schneider et al. [1] has revealed the appearance of oscillations in the energy of topological edge states due to finite size effects. As the size of the spin chain at the origin of the in-gap states changes, the energy of the edge states also changes. This behavior takes place even when the in-gaps states are in a topological phase where they should be robust zero-energy modes. Moreover, the evolution of the oscillations with the system's parameters is very strong and at first sight impossible to predict.

Mier et al. show that this is because two competing spatial frequencies produce a moiré pattern. The moiré is produced by the rapid Friedel-like oscillations due to the spin chain on the superconductor, overlaid by the discreteness of the spin lattice. These two periodicities joined in the complicated way of a moiré leading to the above startling behavior. After this realization, it is simple to predict the periodicity of the ensuing oscillations and to design new spin chains. Indeed, the authors propose a special spin chain for the experimental case mentioned before[1] that shows no oscillations whatsoever.

Thus, this work combines the recent topic of moiré bands with the novelty that these also happen in classical s-wave superconductors. It also yields a precise explanation of the very-recent experiments of Schneider et al., and the prediction that Mier et al. can design edge states with flat dispersion. Thus topological edge states can be studied independently of the foreseeable size distribution of any procedure to fabricate spin chains.

[1] *L. Schneider, P. Beck, J. Neuhaus-Steinmetz, L. R´ozsa, T. Posske, J. Wiebe, and R. Wiesendanger. Precursors of Majorana modes and their length-dependent energy oscillations probed at both ends of atomic Shiba chains. Nature Nanotechnology 17, 384 (2022).*

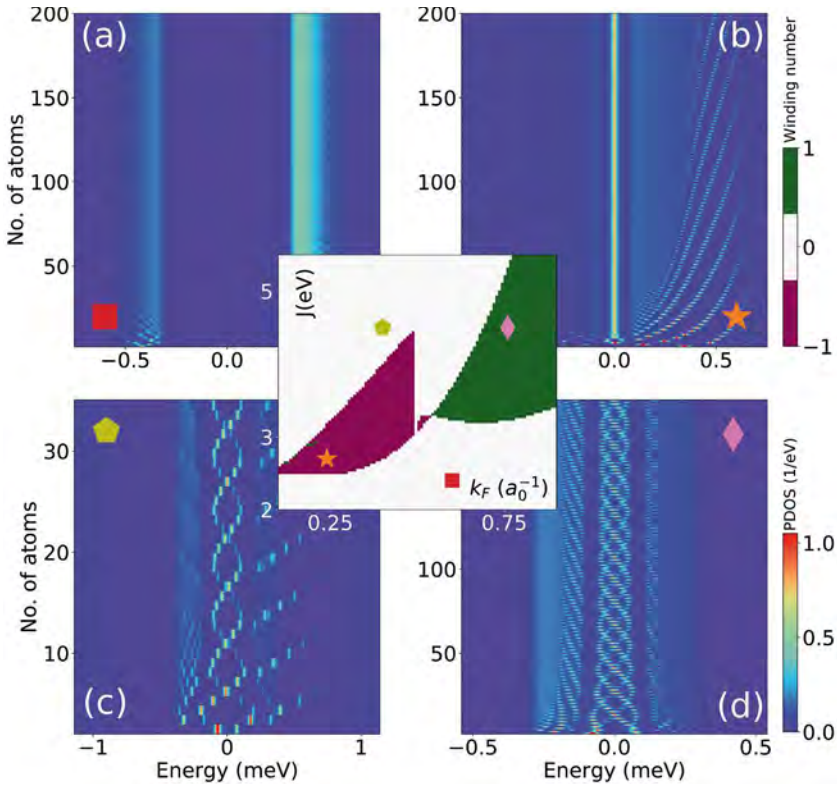


Figure: *Four different behaviors of in-gap states as a function of state energy (x-axis) and spin-chain length (y-axis). The four panels correlate with four different phases in the phase diagram of the inset, where the x-axis is the Fermi wave vector (representative of the superconductor´s electronic density) and the y-axis is the Kondo exchange interaction between the spins and the superconductor's electrons. Red corresponds to a topological phase of widning number +1 and green to winding number -1. The authors show that only for the low density topological region, the Majorana bound states are preserved (b)*

"Edge states of superconductor present energy oscillations with spin-chain length due to the moiré pattern caused by two competing spatial periods reflecting the electronic density and the spin density"

HIGHLIGHT 3 – Nanophysics Lab

Structure matters: asymmetric CO oxidation at Rh steps with different atomic packing

Fernando García-Martínez, Lisa Rämisch, Khadiza Ali, Iradwikanari Waluyo, Rodrigo Castrillo Bodero, Sebastian Pfaff, Ignacio J. Villar-García, Andrew Leigh Walter, Adrian Hunt, Virginia Pérez-Dieste, Johan Zetterberg, Edvin Lundgren, Frederik Schiller, and J. Enrique Ortega

Journal of the American Chemical Society 144, 15363 (2022)

The CO oxidation reaction was monitored operating on a curved rhodium crystal, using Ambient Pressure Photoemission. Maps of surface species obtained within a wide range of temperatures demonstrate a step-packing-dependent asymmetry of the reaction process, proving the persistent presence of very active chemisorbed oxygen at triangular B-type steps.

The carbon monoxide (CO) oxidation ($CO + ½ O_2 \rightarrow CO_2$) is an industrially relevant catalytic reaction, and accordingly, it is among the most studied processes in fundamental surface science. This has led to a wealth of research studies in vacuum, but the doubts remain on whether this reaction proceeds in the same way when changing to realistic conditions. With the advent of powerful analytical techniques that operate at high gas pressures, such as Ambient Pressure X-ray Photoemission (AP-XPS), the "pressure gap" has been reduced significantly. However, a "materials gap" persists, since most AP-XPS studies are carried out using single crystal surfaces, which contrast with the multi-facet structure of technologically relevant nanoparticles.

Curved crystals are a simple approach to bridge the materials gap between single crystal surfaces and nanoparticle catalysts, as depicted in Figure 1. This shows a Rh crystal "curved" around the (111) direction, leading to a smooth variation of the crystal plane at each point. Such geometry allows the different crystal facets to be sequentially probed by scanning the X-ray beam in AP-XPS. With this approach, the authors have

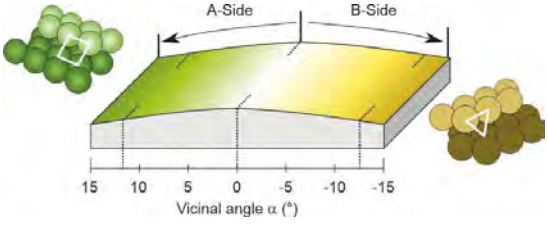


Figure 1: *Schematic description of the curved Rh(111) sample used to probe the catalytic activity of Rh atomic steps with square (A-type) and triangular (B-type) symmetry in a simultaneous way, via Near Ambient Pressure Photoemission.*

"Using a curved crystal sample, surface chemical species appearing during the CO oxidation reaction are imaged across different Rh crystal planes, at different temperatures around the ignition."

investigated the effect of A-type (square geometry, left side of the crystal) and B-type (triangular geometry, right side of the crystal) atomic packing of steps on the catalytic CO oxidation on Rh at millibar pressures.

In this work, researchers from CFM and other institutions from Donostia / San Sebastian together with an international collaboration team have exposed the Rh curved sample of Figure 1 to a reactive CO+O_2 atmosphere, and have identified the sequence and thermal evolution of surface chemical species across the different crystal planes around the reaction light-off. A striking asymmetry is observed between A- and B-type steps both during the ignition and at the fully active reaction stages. Figure 2 shows XPS maps of chemical species at different temperatures as a function of the local crystal plane. The maps acquired during the ignition prove the partial CO-depletion and O-accumulation at B-steps, triggering the earlier B-step ignition. In the active stage of the reaction, the low-active Rh oxide builds up at A-steps (square atomic packing), while B-steps (triangular atomic packing) retain the active chemisorbed oxygen species during reaction conditions.

In this work, the authors improve over a classical trajectory method by including quantum corrections. The interaction between the molecules and the surface are described by density functional theory. They assign statistical weights to classical paths on the basis of two semiclassical corrections: Gaussian binning and the adiabaticity correction.

"Both the ignition process and the active phase exhibit a remarkable A-B asymmetry, with B steps retaining the very active chemisorbed oxygen species at all reaction stages."

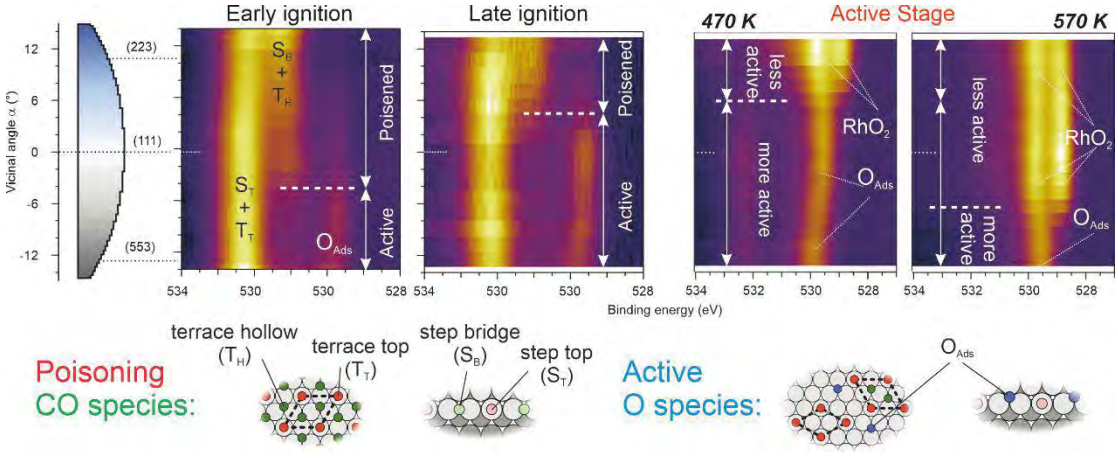


Figure 2: *Map of surface chemical species across different crystal planes (vicinal angle α on the curved Rh(111) sample), measured at near-ambient pressure (0.5:0.5 mbar of CO:O2), at different temperatures around the ignition point and the active stage. A marked A-B asymmetry is observed at all reaction stages.*

HIGHLIGHT 4 – Nanophysics Lab

Solving stability problems of relevant graphene derivatives

James Lawrence, Alejandro Berdonces-Layunta, Shayan Edalatmanesh, Jesús Castro-Esteban, Tao Wang, Alejandro Jimenez-Martin, Bruno de la Torre, Rodrigo Castrillo-Bodero, Paula Angulo-Portugal, Mohammed S. G. Mohammed, Adam Matěj, Manuel Vilas-Varela, Frederik Schiller, Martina Corso, Pavel Jelinek, Diego Peña and Dimas G. de Oteyza.

Nature Chemistry 14, 1451 (2022)

In the last decades, a new synthetic approach has been developed, generally termed as "on-surface synthesis" that substantially departs from standard wet-chemistry. Instead of the three-dimensional space of solvents in the latter, the environment of the reactants in this new approach are well-defined two-dimensional solid surfaces that are typically held under vacuum conditions. These differences have allowed the successful synthesis of a great variety of molecular structures that could not be obtained by conventional means. Among the structures that are raising particular interest, carbon-nanostructures with zigzag-shaped edges are found, which endow the materials with exciting electronic and even magnetic properties of potential interest for a great variety of applications that include quantum technologies.

An important downside of these materials, however, is that they often lack sufficient chemical stability to withstand air exposure. That is why environments like vacuum are used to make the synthesis possible. Unfortunately, for their ultimate implementation in actual devices, these structures need to be manipulated and transferred out of the vacuum, which would degrade the materials and therefore jeopardize their potential utilization. This brings up the need to conceive new strategies for the device fabrication processes. In conventional chemistry, protection/deprotection strategies are commonly applied to overcome stability problems. However, it remained to be tested whether such protection chemistry strategies could also be applied in "on-surface synthesis".

In this work, an international team from DIPC and CFM in Donostia / San Sebastian, CIQUS - Universidade de Santiago de Compostela, Czech Academy of Sciences (Prague), Palacký University (Olomouc), Ikerbasque (Basque Country) and CINN (CSIC-UNIOVI-PA) in El Entrego, performed such tests with narrow stripes of graphene nanoribbons featuring a large density of zigzag-shaped edges. The work presents two related but complementary methods to apply the protection/deprotection strategy to the reactive zigzag edge segments of nanographenes.

In particular, the authors have demonstrated the usage of atomic hydrogen as a means of protecting the nanostructured graphene from the oxidising effects of the atmosphere. Afterwards, the nanostructures were easily dehydrogenated and converted back to their original form via annealing. An alternative approach further allowed them to convert an air-stable, chemically modified form of the graphene nanostructures with protective ketone side groups, into the molecules of interest.

The implications of these results are far reaching. The demonstrated protection/deprotection strategy is expected to be similarly applicable to graphene nanostructures with zigzag edge segments different from those probed here. It thus opens new doors for the conception of approaches to integrate carbon nanostructures into devices and may thereby bring the exploitation of the unique characteristics of their zigzag edges a step closer to scalable applications, a grand scientific challenge that cuts across physics, chemistry, materials science and engineering.

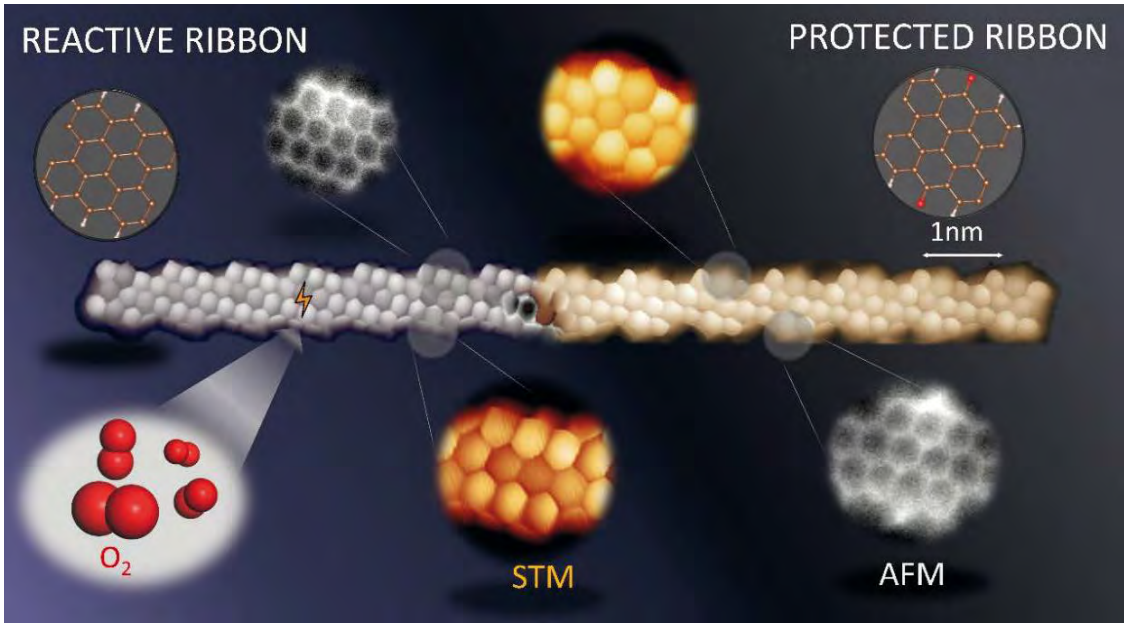


Figure: *Scanning probe microscopy image of a reactive (left) and protected (right) graphene nanoribbon.*

HIGHLIGHT 5 – Modelisation and Simulation

Native point defects and their implications for the Dirac point gap at $MnBi_2Te_4$(0001)

Manuela Garnica Alonso, Mikhail Otrokov, Pablo Casado Aguilar, Ilya Klimovskikh, Dmitry Estyunin, Ziya S. Aliev, Imamaddin Rajabali Amiraslanov, Nadir Abdullayev, Vladimir Zverev, Mahammad Baba Babanly, Nazim Mamedov, Alexander Shikin, Andrés Arnau, Amadeo L Vazquez De Parga, Evgueni VV Chulkov, and Rodolfo Miranda.

NPJ Quantum Materials 7, 7 (2022)

Recently discovered antiferromagnetic topological insulator $MnBi_2Te_4$ represents a fertile platform for realization of numerous quantum phenomena. The characteristic making this material so attractive is its predicted large surface gap. This study reveals an unexpected and dramatic negative effect that $MnBi_2Te_4$'s native defects may have on the size of this gap.

The size of the surface gap of $MnBi_2Te_4$ has been a subject of a fierce debate recently. Density functional theory calculations predict this gap to reach almost 100 meV. However, the experimental studies have reported contradictory results, with some groups finding a gapped surface, in agreement with theoretical predictions, while others revealing practically gapless spectrum. A number of possible theoretical explanations of this unexpected behavior have been put forward, but none of them has been confirmed experimentally.

In this paper, the authors report on a combined study of the $MnBi_2Te_4$(0001) surface using low-temperature scanning tunneling microscopy/spectroscopy (STM/S), high-resolution micro(μ)-laser angle-resolved photoemission spectroscopy (ARPES), and density functional theory calculations. High-resolution STM topographs complemented by the STM simulations allow the team to identify a presence of an intermixing between Mn and Bi sublattices of the material (Figure 1a).

The appearance of the Mn-Bi intermixing causes deviations of the magnetic structure from the ideal antiferromagnetic to a ferromagnetic one, in which the local moments of the MnBi defects are coupled antiparallel to those of the central Mn layer. The STS measurements further reveal that, depending on the sample cleavage, the local density of states is compatible with both large (~50 meV) and small (<20 meV) gaps (Figure 1c and e), in agreement with the laser-ARPES experiments, detecting that the gap changes from sample to sample (Figure 1b and d).

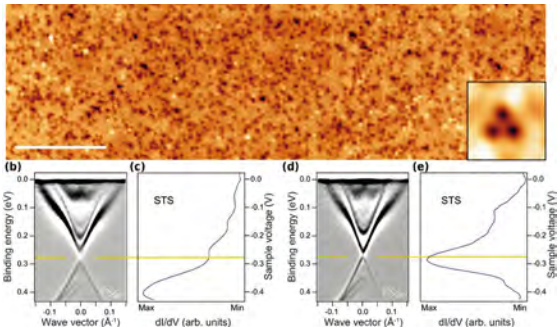


Figure 1: *(a) STM image of a representative area where the characteristic second layer defects (Mn_{Bi}) indicative of the Mn-Bi intermixing can be observed (1 V and 0.1 nA, scale bar 25 nm). Inset: Zoom of 2.5 nm^2 of one of the Mn_{Bi} defects taken at 1 V and 0.1 nA. (b, d) Measured $MnBi_2Te_4$(0001) ARPES dispersions corresponding to a larger (b) and smaller (d) gaps (measurements conditions: photon energy **hv** = 6.3 eV; temperature **T** = 10 K). Note that the second-derivative (d^2**N**/d**E**^{2}) representation of the photoemission data is shown. (c, e) Spatially averaged tunneling conductance spectra showing a clear dip (c) and peak (e) at the expected energy position of the gap center. The spectra shown in (c, e) are compatible with larger (~50 meV) and smaller (<20 meV) gaps, respectively. The horizontal yellow lines show the correspondence between the ARPES and STS spectra. The ARPES data in (b) and (d) correspond to two different samples, while the STS data in (c) and (e) have been acquired from yet another sample, but after different cleavages.*

These surface electronic structure calculations show that the MnBi defects cause a strong reduction of the $MnBi_2Te_4$ surface gap due to the antiparallel alignment of the MnBi moments with respect to those of the Mn layer and predominant localization of the topological surface state near the Bi layers (Figure 2). We thus attribute the variation of the surface gap in the same sample (as observed by STS) or different samples (ARPES) to a different degree of the defectness of the $MnBi_2Te_4$ crystals at local or global structure level, respectively. These results are instrumental in unifying seemingly contradictory reports concerning the $MnBi_2Te_4$ surface gap and stress a necessity of suppressing the cation (Mn-Bi) intermixing thus reducing the number of the MnBi defects in this antiferromagnetic topological insulator.

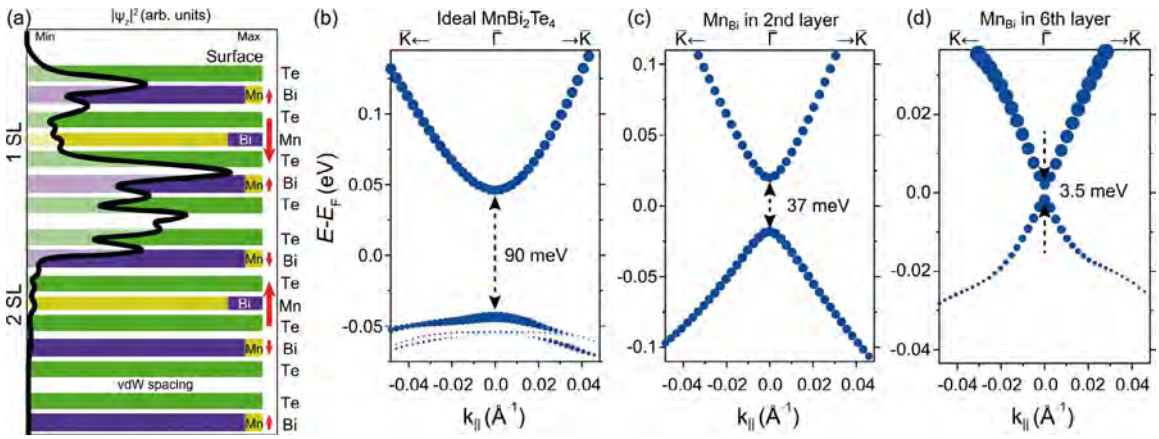


Figure 2: *(a) Illustration of the topological surface state real space distribution at the $MnBi_2Te_4$(0001) surface. The $|\Psi z|^2$ profile corresponds to the band structure shown in panel (b). The Mn-Bi intermixing leads to the appearance of the Mn_{Bi} magnetic moments in the Bi layers that are coupled antiparallel to those in the central Mn layer of the same septuple layer (SL). The Mn_{Bi} magnetic moments thus turn out to be located in the regions with a high weight of the topological surface state, strongly counteracting the effect from the magnetization of the central Mn layer, where the topological surface state weight is low. This is expected to lead to a strong reduction of the surface gap. The latter is illustrated in panels (b–d), where the $MnBi_2Te_4$ surface electronic structure in the defectless case (b) is compared to those with Mn-Bi intermixing when Mn_{Bi} defect locates in the second (c) and sixth (d) atomic (i.e., Bi) layers counting from the surface (see (a)). Note that only the topological surface state is shown, while the bulk-like bands are omitted. The energy axes scales in (b, c) and (d) are different.*

Empowering non-covalent hydrogen, halogen, and $[S–N]_2$ bonds in synergistic molecular assemblies on Au(111)

Ana Barragán, Sara Lois, Ane Sarasola, and Lucia Vitali

Nanoscale (2022), 14, 17895

The concept of synergy is important in organic materials, as molecules self-assemble into characteristic molecular synthons through multiple non-covalent interactions. The resulting cohesion energy is non-additive and greater than the sum of the individual bond interaction. Two distinct networks formed by 2Br-BTD molecules on Au(111), here reported, perfectly describe this cooperative contribution.

Non-covalent intermolecular bonds are fundamental in self-assembled organic structures. Although weak in nature, these secondary-bonding interactions act on long-range between molecular regions with positive and negative potentials leading to highly-directional bonds. Consequently, characteristic arrangements of interacting molecules, called synthons, shape the crystal structure, define the charge transport and the catalytic properties, and are fundamental in drug design and in biochemistry. However, the most interesting thing is that these weak interactions allow for crystal design and engineering of its specific electronic, mechanical, and lattice dynamic properties under mild conditions. Although these interactions are of interest for fundamental studies and for applied optoelectronics such as photovoltaics, photoluminescence, sensing, organic-based electronics, or medical diagnostics, very few works have addressed their synergistic role. Indeed, very often, these interactions are masked by strong covalent bonds in metal–organic assemblies, or by the interaction with the supporting metal surfaces.

This collaborative work addresses the synergistic action of multiple secondary bonds. By means of scanning tunneling microscopy (STM) and density functional theory (DFT), the authors have characterized the assembling of one molecular specie, namely 4,7-dibromobenzo[c]-1,2,5-thiadiazole

(2Br-BTD), in two different patterns on the Au(111) surface. Intermolecular interactions with high directionality determine the pattern of two different networks by forming distinct molecular synthons. This structure tunability shows the easiness of the structural adaptability of non-covalent interactions. Both structures exhibit a distinct synergistic contribution that causes the cohesive energy of the system to increase in a nonadditive way. Barragan et al. found that the $[S–N]_2$ synthon, a common feature of the two structures and certainly one of the driving forces of the assembly, benefits the most from this cooperative action, despite the fact that they observed a significant reduction of other 3 to 4 interatomic distances, such as N–H, Br–Br, and Br–H, with respect to the isolated synthon. Yet, due to steric hindrance, not all these nodal structures contribute to the cohesive energy of the system. Whenever this occurs, other secondary bonds involving hydrogen or nitrogen compensate for the eventual deficiency.

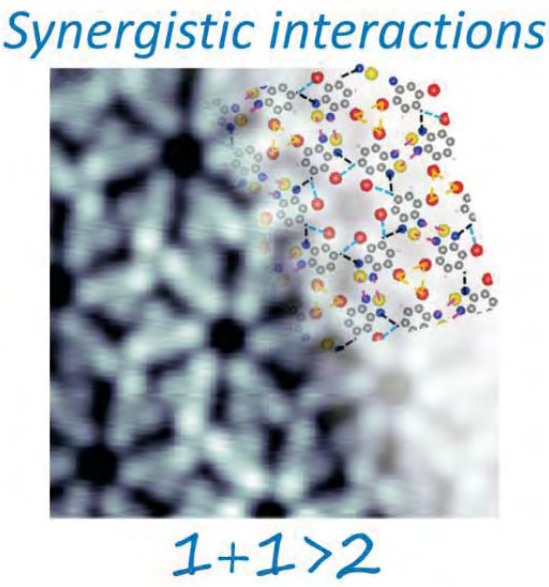


Figure: *Graphical representation of the multiple non-covalent bonds involved in the assembly of one of the two crystal structures of 2Br-BTD molecules on Au(111).*

Parallel versus twisted pentacenes: conformational impact on singlet fission

Ilias Papadopoulos, S. Rajagopala Reddy, Pedro B. Coto, Dan Lehnherr, Dominik Thiel, Michael Thoss, Rik R. Tykwinski, and Dirk M. Guldi.

Journal of Physical Chemistry Letters 13, 5094 (2022)

In this work, the authors placed two pentacene chromophores at the termini of a diacetylene linker to investigate thez impact of excitation wavelength, conformational flexibility, and vibronic coupling on singlet fission. The results highlight the need of controlling the emergence of twisted conformations in the design of new singlet fission active molecules.

Harnessing triplet excited states (T1) in up/down converting solar energy processes in single-junction solar cells has proven a useful tool to maximize the use of the solar spectrum, introducing also ways to overcome the Shockley–Queisser efficiency limit. In this context, multiple exciton generation in semiconductor materials and singlet fission (SF) in molecular materials are promising candidates to maximize the efficiency of solar cells. Here, Papadopoulos et al. have synthesized LiDi, a diacetylene linked pentacene dimer, to assess the impact that conformational flexibility, excitation wavelength, and vibronic coupling have on the intramolecular SF (iSF) mechanism. Steady-state absorption measurements reveal vibrational splitting, inferring the existence of at least two types of conformers, in which the pentacene moieties are placed either parallel or twisted with respect to each other. Using time-resolved transient absorption spectroscopy, they have analyzed the low- and high-energy transitions of LiDi. Photoexcitation of the low-energy transitions identifies a superposed mixture of states, which transforms into a single observable species, namely a delocalized vibronically coupled/hot triplet pair 1(T1T1) deloc with a short lifetime (< 2 ps). Photoexcitation of the high-energy transitions of LiDi, on the other hand, results in the observation of a superposed mixture of states and its transformation into 1(T1T1) deloc within 1.0 ps. This state decays to the ground state within 4 ps via triplet–triplet annihilation. Lowering the temperature allows the

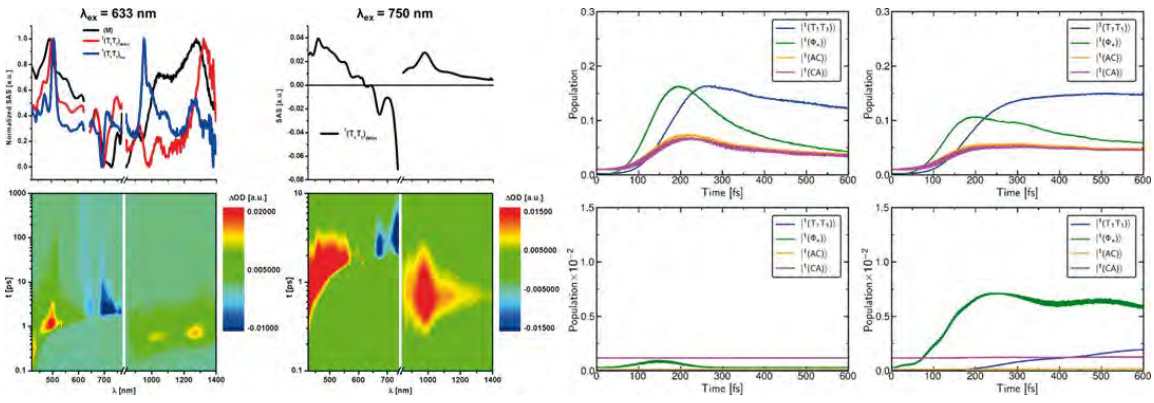


Figure: *Left- Differential femtosecond transient absorption spectra of LiDi in MeTHF at 80 K with λex 633 and 750 nm, respectively. The upper panel shows the respective species associated spectra of the mixed state (M) (black), the delocalized and vibronically coupled/hot 1(T1T1)deloc (red), and the localized and vibronically decoupled 1(T1T1)loc (blue) as obtained by target analysis. Right- Simulated time evolution of the population of the diabatic states involved in the iSF process of LiDi (top) and twisted LiDi (bottom) conformers after photoexcitation at 717 nm (left) and 659 nm (right) correlating with the experimentally used excitation wavelengths.*

identification of two different correlated triplet-pair excited states, with different spectroscopic features. The authors relate these states to the delocalized 1(T1T1) deloc and to a localized and vibronically decoupled 1(T1T1)loc state, respectively. Quantum dynamics simulations are consistent with an iSF dominated by the mediated-like mechanism and excitation-wavelength-dependent on short time scales (ca. < 10 ps). In addition, theory suggests that the quasi-free rotation at the diacetylene spacer exhibited by LiDi may easily lead to twisted conformations with very low SF quantum yields.

Altogether, these results emphasize the necessity of controlling conformational flexibility in the design of new SF-active materials.

HIGHLIGHT 8 – Electronic Excitations in Surfaces and Nanostructures

Rashba-like physics in condensed matter

Gustav Bihlmayer, Paul Noël, Denis V. Vyalikh, Evgueni V. Chulkov and Aurélien Manchon.

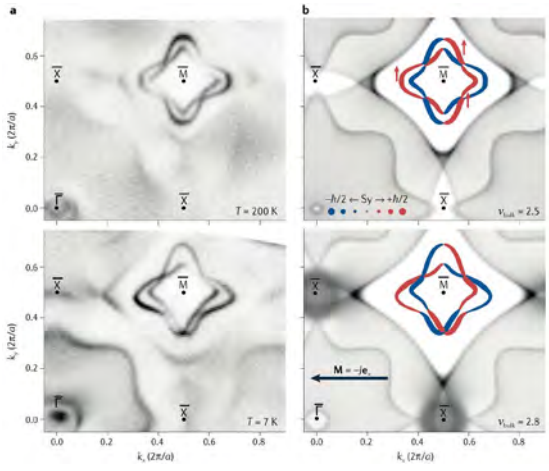
Nature Reviews Physics 4, 642 (2022)

Spin–orbit coupling induces a unique form of Zeeman interaction in momentum space in materials that lack inversion symmetry: the electron's spin is locked on an effective magnetic field that is odd in momentum.

The resulting interconnection between the electron's momentum and its spin leads to various effects such as electric dipole spin resonance, anisotropic spin relaxation and the Aharonov–Casher effect, but also to electrically driven and optically driven spin galvanic effects. Over the past 15 years, the emergence of topological materials has widened this research field by introducing complex forms of spin textures and orbital hybridization. The vast field of Rashba-like physics is now blooming, with great attention paid to non-equilibrium mechanisms such as spin-to-charge conversion, but also to nonlinear transport effects. This Review aims to offer an overview of recent progress in the development of condensed matter research that exploits the unique properties of spin–orbit coupling in non-centrosymmetric heterostructures.

A few keypoints:

- The Rashba effect is a mechanism that locks the spin of a charge carrier to its momentum and stems from the coexistence of inversion symmetry breaking and spin–orbit coupling.
- The Rashba effect is ubiquitous in condensed matter and exists in a wide variety of systems and heterostructures, including semiconductors, metals, superconductors and correlated materials.
- The physics of the Rashba effect is at the origin of several important phenomena in condensed matter, including spin-to-charge interconversion, non-reciprocal magnetoelectric and magnetoptical response, and anomalous nonlinear effects.
- Depending on the crystal and magnetic symmetries of the system under consideration, complex forms of spin–momentum locking and dispersion can be obtained, leading to a rich zoo of phenomena.



"The impact of the Rashba effect extends far beyond spin transport and is at the basis of several key concepts in topological insulators, semimetals and superconductors."

Figure: *Cubic Rashba effect and emergence of 2D ferromagnetism at iridium silicide surface of valence-fluctuating $EuIr_2Si_2$. a) Fermi surface at 200 K (upper panel) and 7 K (lower panel). The results are derived from angle- resolved photoemission spectroscopy (ARPES). b) The computed Fermi surface for 200 K (upper panel) and 7 K (lower panel), shown as a superposition of projected bulk and slab- derived states calculated within density functional theory. The surface state is highlighted by the spin expectation value Sy in red (Sy > 0) and blue (Sy < 0). The black arrow indicates the direction of the emergent magnetic field.*

Theory of the supercurrent diode effect in rashba superconductors with arbitrary disorder

Stefan Ilic, and F. Sebastian Bergeret.

Physical Review Letters 128, 177001 (2022)

The diode effect in superconductors attracts great interest for its promising applications in superconducting electronics. Furthermore, this effect is predicted to be observed in helical superconductors, i.e., superconductors with strong spin-orbit coupling and an exchange field.

Almost all previous theoretical works only considered ballistic transport in ideally clean superconductors. In this work, the authors demonstrate how the diode effect survives disorder and can be expected to be observed in real materials.

The interplay between superconductivity, spin-orbit coupling (SOC), and a Zeeman field leads to a variety of magnetoelectric effects widely studied in the past years. One of these effects is a nonreciprocal charge transport due to the breaking of time-reversal and inversion symmetries. Nonreciprocity manifests, for example, in the supercurrent in noncentrosymmetric superconducting structures and in Josephson junctions. The critical current depends on the direction of the current flow: by tuning the amplitude of the current between the two critical values the system will behave as a normal conductor in one direction and as a superconductor in the other. Such systems are being suggested as superconducting diodes with potential applications in low-power logic circuits.

All previous theoretical works assume ideally pure superconducting structures and disregard the effect of disorder. However, disorder is unavoidable in realistic structures, and therefore it is important to understand how it affects the supercurrent diode effect. In this work, the team establishes the microscopic theory of the supercurrent diode effect in disordered two-dimensional Rashba superconductors.

These results elucidate the mechanisms leading to the diode effect, and show how it evolves in the full range of all relevant system parameters: SOC, magnetic field, temperature, and disorder. Namely, the effect stems from the competition between two helical bands in a Rashba super- conductor, which prefers opposite modulation vectors of the superconducting order parameter when magnetic field is applied. Both magnetic field and SOC are required for the diode effect; however, if either is too strong, the band competition

HIGHLIGHT 9– Mesoscopic Physics

ceases as one helical band begins to dominate, leading to the suppression of the effect. This means that a substantial diode effect exists only for some optimal magnetic field and SOC. Disorder further complicates this picture, as it introduces mixing of the two helical bands. illic et al. discuss optimal parameter regimes where the effect is strongest and establish that the effect persists even at strong disorder. Moreover, this work shows that the sign of the rectification changes by increasing the disorder. The change of sign can be related to the change of nature of the helical phase.

"The change of sign of the diode effect can be related to the change of nature of the helical phase of the superconductor"

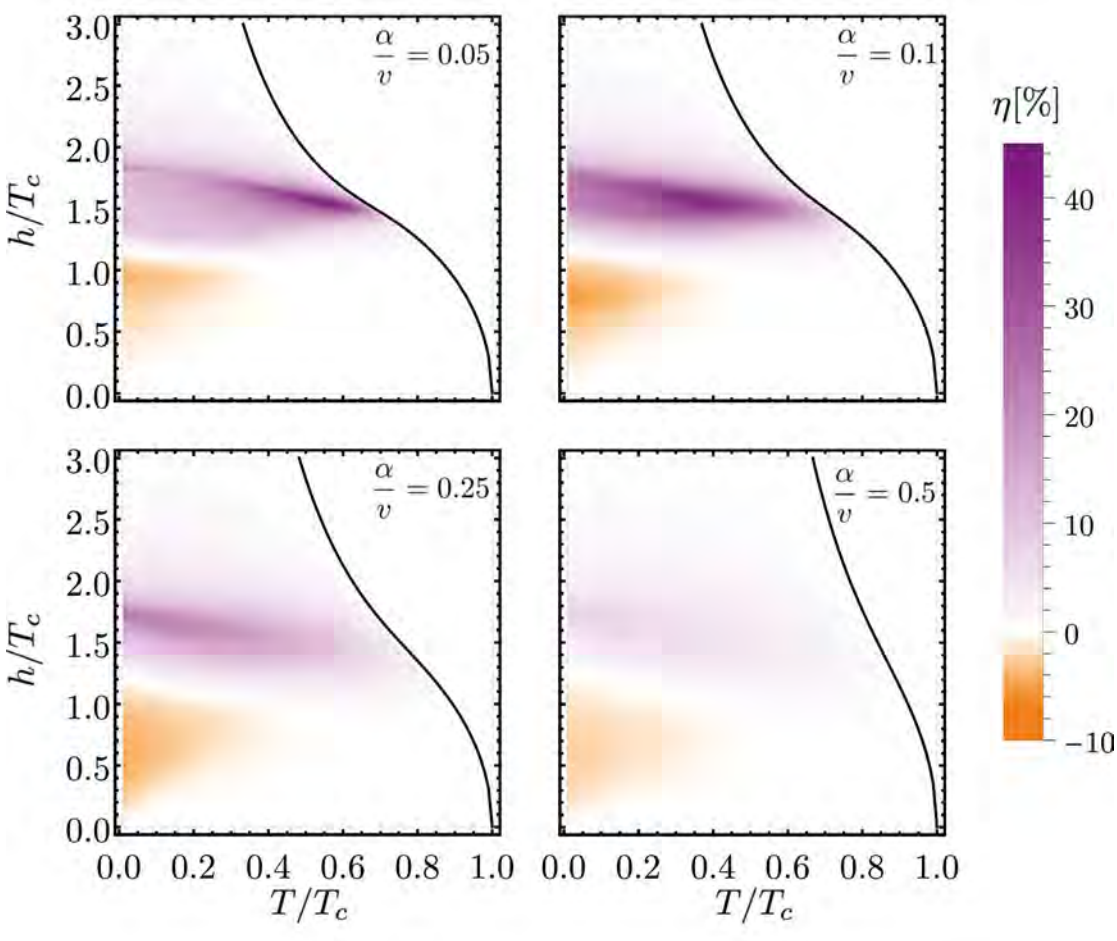


Figure: *The diode quality factor calculated for every point in the Zeeman field (h)– Temperature (T) phase diagram at different strengths of spin-orbit coupling.*

Cementitious materials as promising radiative coolers for solar cells

Matteo Cagnoni, Alberto Tibaldi, Jorge S. Dolado, and Federica Cappeluti.

iScience 25 (2022) 11, 105320

Over the years, researchers have developed several cooling technologies for photovoltaic systems, to take advantage of the enhanced power conversion efficiency and extended system lifetime provided by a reduced operating temperature. Recently, radiative cooling has been drawing significant attention as a potentially efficient and cost-effective solution for the thermal management of solar cells, able to satisfy energetic, economic and environmental needs without compromising system simplicity. Unfortunately, the radiative coolers proposed so far rely on metamaterials based on expensive elements, complex fabrication processes, or organic polymers with possible UV-degradation.

Researchers of the MIRACLE consortium are trying to eliminate these weaknesses by efficient radiative coolers based on cheap, scalable and robust cementitious materials. Indeed, in this work from the *Politecnico di Torino* and CFM, Cagnoni et al. have developed a multi-scale interdisciplinary simulation workflow to show for the first time that humble **ordinary Portland cements (OPC) can be equipped with electromagnetic properties suitable for radiative cooling applications**. Furthermore, they have found that the thermodynamic limit of this solution for the thermal management of **solar cells** is a **temperature reduction of about 20 K**, which could correspond to outstanding efficiency and lifetime gains (up to 9% and 4%, respectively).

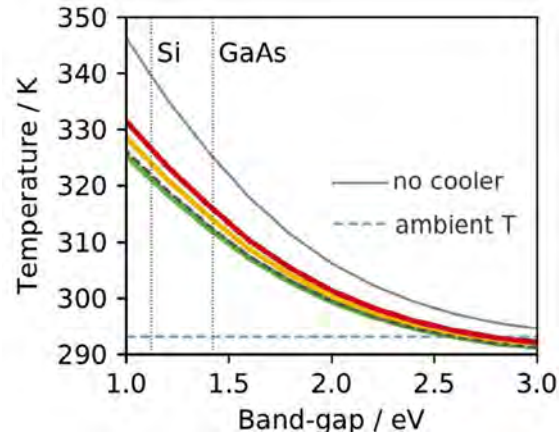


Figure: *Operating temperature as a function of the solar cell semiconductor band-gap with cement-based radiative coolers and nsso cooler. The temperature is reduced by about 20 K in silicon-based devices.*

Their work represents a first step toward the realization of a novel class of radiative coolers based on cementitious materials, combining energetic, economical, reliability and scalability requirements, and is expected to trigger many follow-up studies aimed at achieving the practical realization of this attractive concept.

For more information, visit the MIRACLE web page **miracle-concrete.eu**.

"**Concrete** solutions for improving solar cell efficiency"

HIGHLIGHT 11 – Theory of Nanophotonics

Mapping Lamb, Stark, and Purcel effects at a chromophore-picocavity junction with hyper-resolved fluorescence microscopy

Anna Rosławska, Tomáš Neuman, Benjamin Doppagne, Andrei G. Borisov, Michelangelo Romeo, Fabrice Scheurer, Javier Aizpurua, and Guillaume Schul.

Physical review X 12, 011012 (2022)

The properties of molecular transitions depend on their optical interaction with the surrounding environment. Confining light to atomic-sized hot spots pushes this effect to its ultimate limit, enabling the characterization and control of the energy and losses of a molecular transition with submolecular resolution.

The interaction of photons with excitonic and vibrational molecular transitions is often the target of state-of-the-art spectroscopic and microscopic techniques. This interaction can be enhanced by using optical nanoresonators that confine electromagnetic energy into tiny volumes of space. Plasmonic modes in metallic nanocavities are particularly attractive in this context, since they push light confinement to the limit as compared to standard dielectric resonators.

Confinement of photons in nanocavities enables to obtain optical images of molecular excited states with improved resolution. The characterization of different regions of the excitations in individual molecules (submolecular resolutions), is, however, a formidable challenge, only recently surmounted with the use of plasmonic picocavities in Scanning Tunnelling Microscopy (STM) configurations. Picocavities are created by atomistic features in an STM tip, strongly boosting electromagnetic fields in atomic-sized regions.

A theoretical and experimental study developed in a collaboration by the Theory of Nanophotonics group in CFM, the tunnelling microscopy group at the University of Strasbourg, and researchers at University Paris-Saclay, has demonstrated and interpreted submolecular resolution with the use of a picocavity not only in the optical characterization, but also in the manipulation of the properties of excitonic molecular transitions. As the tip of a STM is placed over different positions on top of a phthalocyanine molecule, a strong change of the energy and decay rate (effective losses) of an excitonic transition of the molecule is measured. The increase of the decay rate is produced as a consequence of the optical coupling between the plasmonic picocavity and the molecule (Purcell effect).

Understanding the changes of the transition energy induced by the tip position requires to consider both the electrodynamical coupling (Lamb shift) as well as the electrostatic interaction (Stark shift). This work thus emphasizes the exquisite control of the optical properties of single molecules achievable in STM, as well as the subtle origin of some of the spectroscopic and microscopic features.

"Intramolecular resolution of light emission by a single molecule is achieved by an STM picocavity"

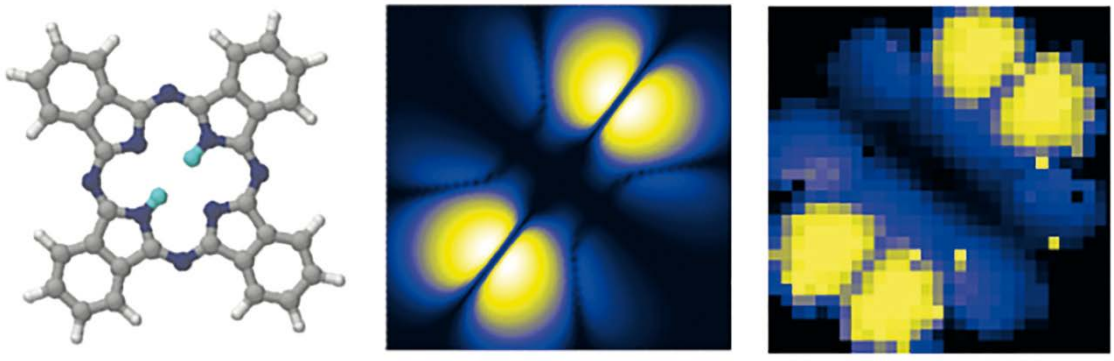


Figure: *Left: Structure of the free-base phthalocyanine (H2Pc) molecule. Center: Experimental map of light emission from the H2Pc molecule deposited on an NaCl-Ag(111) surface when scanned in a STM picocavity. The area of scanning is 2.5 x 2.5 nm2, and the bias voltage applied is V=-2.5 V, with a current I= 100 pA. Right: Theoretical map of light emission under the same circumstances as in the experiment. The spectral range of light emission considered is at the excitonic emission line ~1.975 eV.*

Cross determination of exciton coherence length in J-aggregates

Alba María Jumbo Nogales, Victor Krivenkov, Konstantin Rusakov, Alexander S.Urban, Marek Grzelczak, and Yury Petrovich Rakovich.

Journal of Physical Chemistry Letters 13, 10198 (2022)

The coherence length of the excitons N is a critical parameter governing key features of J-aggregates. Determining N is a nontrivial task since it is sensitive to the technique applied, causing many reported discrepancies. By using a combination of different experimental techniques Jumbo-Nogales et al. determined N values in a wide range of pH.

J-aggregates are self-assembled supramolecular structures constituting organic molecules, organized into quasi-1D chains. Strong in-line dipole−dipole coupling in these systems leads to the generation of the Frenkel exciton, and coherence of the exciton wave function across several interconnected monomer units rendering a narrow absorption band (redshifted with respect to monomer)-the so-called J-band. A quantitative description of long-range exciton migration involves the determination of coherence length N (or the exciton coherence length). It tells about the number of molecules of an aggregate over which the exciton wave function is coherent, the dipole momentum, oscillator strength, and the radiative lifetime of the exciton transition. The coherence length also has some implications for the nature of long-distance exciton migration and transport and for research on strong light−matter interaction.

In this paper, the authors quantify the coherence length of cyanine dye as an exemplar model J-aggregates system. The excitonic properties of organic J-aggregates were studied using several different spectroscopic techniques: absorption and transient absorption spectra, and PL spectra and PL lifetimes. This work shows that a correct and reliable determination of the exciton coherence length requires a careful and comprehensive approach. This cannot be done using single-experimental analysis at fixed experimental conditions.

By using a combination of different experimental techniques including UV−vis−NIR, fluorescence emission,

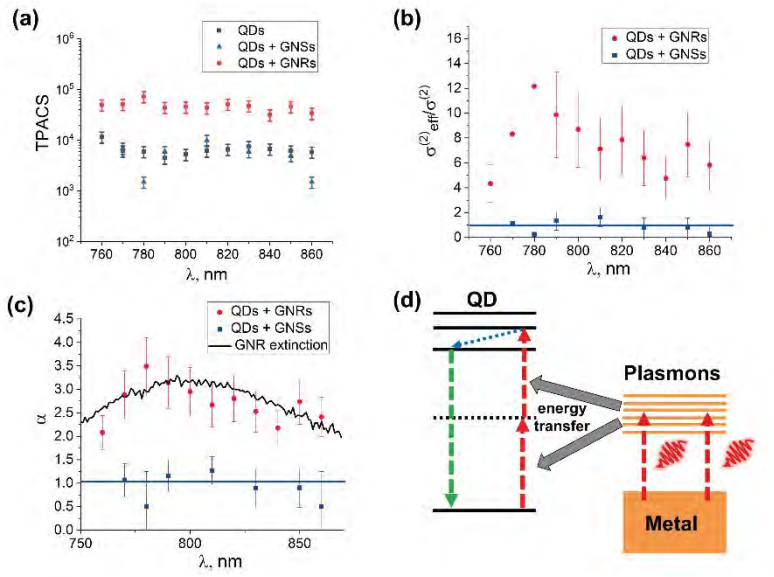


Figure: *Effect of gold nanorods on the Two-Photon Absorption Cross-Sections (TPACS) of excitons in semiconductor Quantum Dots (QDs). a) The measured TPACS of excitons in QDs in the absence of plasmon nanoparticles (black squares), QDs near gold nanospheres (blue triangles), and QDs near gold nanorods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

time-resolved photoluminescence, and transient absorption spectroscopies, they determined N values for J-aggregates of a cyanine dye in a self-consistent way. It was found that the absorption spectroscopy alone - a widely used technique- fails in determining right value for N. The correct approach is based on the modification of photoluminescence lifetime and nonlinear response upon aggregation and careful analysis of the Stokes shift and electron–phonon coupling strength. This approach revealed that N of JC-1 J-aggregates ranges from 3 to 6.

The analysis of all the data obtained from each one of the mentioned techniques allowed to build a better picture of the aggregation process and the excitonic behavior in the monomer chains. Finally, the calculated parameters are presented to quantify these J-aggregate properties in order to strengthen their current applications and to help develop new ones.

HIGHLIGHT 13 – Laser Physics and Photonic Materials

Dehydroxylation processing and lasing properties of an Nd alumino-phosphate glass

Mónica Muñoz-Quiñonero, Jon Azkargorta, Ignacio Iparraguirre, Rafael J. Jiménez-Riobóo, Gregory Tricot, Chongyoun Shao, Francisco Muñoz, Joaquín Fernández, and Rolindes Balda.

Journal of Alloys and Compounds 235, 118035 (2022)

The main high energy high power laser phosphate glasses use Nd^{3+} ions as dopant. To determine the suitability of a Nd^{3+}-doped glass laser, a knowledge of the spectroscopic properties are required. In particular, the emission cross-section and the quantum efficiency determine the stored energy in the $^4F_{3/2}$ state and extraction characteristics. Non-radiative processes, if present, reduce the lifetime which leads to a reduction of the stored energy and affect the output laser energy. As energy transfer to OH vibrational modes is an important source of non-radiative losses in these Nd-doped glasses, dehydroxylation of the phosphate glasses is of paramount importance to achieve a good laser performance.

In this collaborative work carried out by the groups led by Alicia Durán (ICV-CSIC) and Rolindes Balda (CFM, UPV/EHU), an aluminophosphate glass composition was selected to carry out a study on the influence of the processing parameters over the dehydroxylation of the glasses, i.e. temperature and time of remelting under N_2, viscosity and mass of glass. The glass composition, $13Na_2O$-$13K_2O$-$16BaO$-$4Al_2O_3$-$54P_2O_5$ (mol %), is close to the available commercial phosphate laser glasses for high power lasers such as LG-750, LG770, or LHG-8. Laser experiments were performed using a 5 mm thick plate-shaped sample doped with 2.5 wt% Nd_2O_3 concentration placed at the center of a 10 cm long confocal symmetrical resonator and oriented at Brewster angle with respect to the resonator axis (Figure 1).

The stimulated emission cross-section calculated from spectral data gives a value of 3.9×10^{-20} cm^2, similar to the one of LG-770 (Shott) glass, in reasonably good agreement with the value estimated from laser threshold data ($4 \pm 0.5 \times 10^{-20}$ cm^2). The obtained values for the stimulated emission cross-section, figure of merit (144.3×10^{-25} cm^2s), and quantum efficiency (89%) together with the threshold energy and slope-efficiency of the laser emission at around 1055 nm demonstrate the suitability of this glass for optical amplification (Figure 2). Moreover, the laser emission undergoes detectable changes when the excitation wavelength is tuned along the $^4I_{9/2} \rightarrow {}^4F_{5/2}$ pump band due to the crystal field site effects.

The observed behavior can be explained if the existence of two distributions of sites for the Nd^{3+} ions overlapped in energy is taken into account; one of them very wide but with smaller effective cross-section than the other one located close to the center of the former, whose effective-cross section is larger and sharper. The presence of P-O-Al bonds in the glass network could explain the existence of two broad sites distributions for the rare earth in this glass matrix.

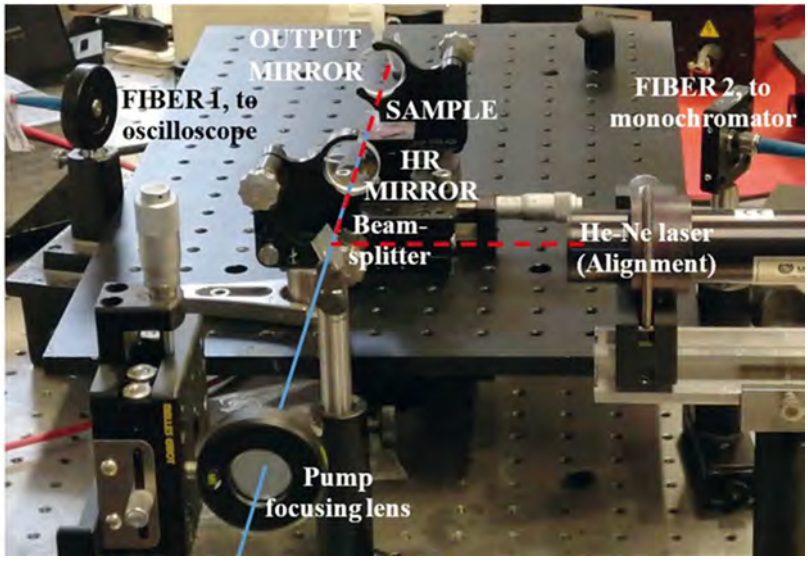


Figure 1: *Experimental set-up used for laser experiments. The sample is located at the center of a confocal resonator consisting in two concave mirrors of curvature radii 10 cm, one HR and an output coupler of reflectivity 70%. The pump beam is addressed collinear to the resonator axis.*

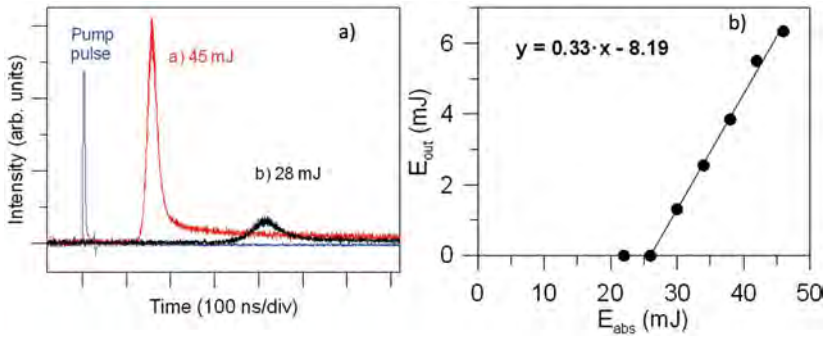


Figure 2: *a) Time-evolution of stimulated emission pulses in $Nd3^{+}$ doped alumino-phosphate glass at two different pump energies. The pump pulse (802 nm wavelength) is at left side of the graph: Black line 28 mJ pump energy, red line 45 mJ pump energy. b) Laser emission energy as a function of pump energy at 802 nm. The threshold energy is 26 mJ and the slope-efficiency is 33 %.*

Validity of effective potentials in crowded solutions of reversible network-forming polymers

Mariarita Paciolla, Christos N. Likos, and Angel J. Moreno.

Macromolecules 55, 2659 (2022)

By combining large-scale simulations and liquid state theory, the authors find that the effective fluid approach provides an excellent description of the structural correlations in reversible polymer networks even in highly crowded conditions. This is a very unusual result in macromolecular solutions, and it is a consequence of the molecular size being unperturbed through reversible intermolecular bonding. Moreover, this results suggests that experimental interpenetrated networks are out-of-equilibrium states where demixing is prevented through dynamic arrest.

The effective potential between two macromolecules separated by a given distance is the free energy needed to bring them from infinity to that distance. Unlike in hard-core colloids, the free energy cost for full interpenetration is finite because their centers-of-mass can coincide in space. This cost strongly depends on their topology and internal deformability, typically varying between a few and tens of times the thermal energy. Averaging out the molecular degrees of freedom and keeping a few relevant coordinates (usually the centers-of-mass) reduces the system to an effective fluid of ultrasoft particles interacting through the effective potential. This methodology allows not only for simulating much larger scales than in the all-monomers system but also for the treatment of the system by methods from liquid state theory, producing a powerful tool to predict large-scale organization and phase behavior. This approximation works below and even slightly above the overlap concentration, (the concentration at which the mean intermolecular distance is of the order of the unperturbed molecular size). However, it fails dramatically far above the overlap concentration when many-body effects become a dominant contribution (shrinkage of the molecular size under crowding being a well-known manifestation of them).

By means of large-scale simulations, Paciolla et al. have systematically derived effective potentials for polymers with reversible bonds, which in crowded conditions can form dynamic networks with viscous flow and self-healing properties. The authors have compared the static correlations in the effective fluid and in the all-monomers system. Rather surprisingly, an excellent agreement is found even far above the overlap concentration. This is consistent with the fact that shrinking is highly prevented by forming intermolecular bonds with neighboring chains, which unlike in crowded polymers without bonds, makes the conformations

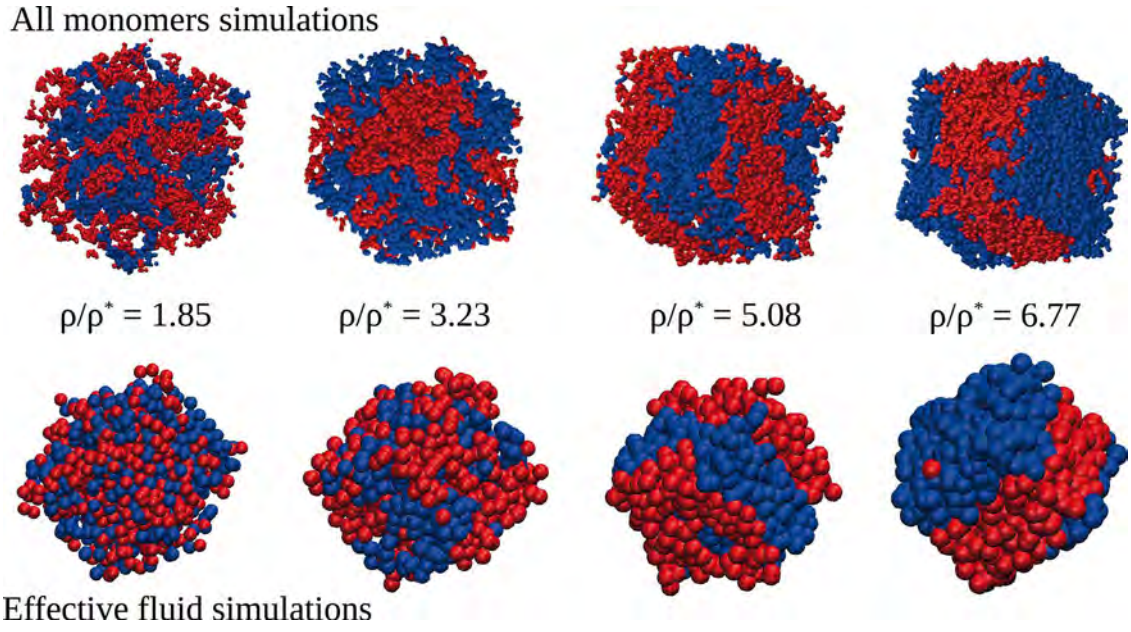


Figure: *Snapshots of the all-monomers system (AM, upper row) and the effective fluid (EF, bottom row) of a binary mixture of polymer chains with orthogonal reversible bonding. The beads represent the actual monomers in the AM case and the effective ultrasoft particles in the EF. Molecules belonging to different components of the mixture are represented by different colors. Demixing is evident in both the AM and EF simulation. Concentrations (ρ) are given in terms of the overlap concentration (ρ*) and correspond to highly crowded conditions.*

weakly sensitive to crowding and many-body effects basically contribute as a flat energy landscape.

Finally, this work explored the possibility of forming two interpenetrated networks in a polymer mixture where the reactive sites of the two components are orthogonal; i.e., intermolecular bonds only occur between chains of the same component. In agreement with the energetic penalty found for the effective cross-interaction potential and the phase diagram predicted for the effective fluid, no interpenetrated networks are found in the all-monomers solutions. Instead, the two components phase separate (demixing), as can be seen in the figure. This result suggests that experimental interpenetrated networks, where both the bond lifetimes and the intrinsic diffusion times of the polymers are much longer than in the simulations, are actually kinetically trapped states with large entropic barriers impeding the relaxation to the equilibrium demixed state.

"The work explores the application of effective potentials to describe structural correlations in dynamic polymer networks"

HIGHLIGHT 15 – Polymers and Soft matter

Disentangling component dynamics in an all-polymer nanocomposite based on single-chain nanoparticles by means of quasielastic neutron scattering

Jon Maiz, Ester Verde-Sesto, Isabel Asenjo-Sanz, Lucile Mangin-Thro, Bernhard Frick, José A. Pomposo, Arantxa Arbe, and Juan Colmenero

Macromolecules 55, 2320 (2022)

One of the first envisaged applications for Single-Chain Nano-Particles (SCNPs) was as 'fillers' of nano-composites due to the tunability of their size, interactions and dynamic asymmetry with the matrix. Unveiling the mutual influence of the components at a microscopic level is a challenge that can be faced by Quasielastic Neutron Scattering (QENS) techniques together with isotopic labeling.

This combination was applied to an all-polymer nanocomposite consisting of 25% SCNPs in a 75% polymer matrix composed by the linear precursor chains of the SCNPs. Two spectrometers were combined to cover a wide dynamic range and properly characterize the complex dynamics of both components in the mixtures. In the raw materials –investigated as reference--, the intra-molecular crosslinks induce a slowing down and a broadening of the dynamic response of the SCNPs with respect to the reference precursors. Dynamic asymmetry is also patent in the nanocomposite. The QENS experiments revealed the development of a dynamic heterogeneity in the nanocomposite components, which grows with increasing time: while the picosecond dynamics of precursor and SCNPs are very similar, they become more and more distinct at longer times. The more retarded dynamics of the SCNPs with respect to the linear chains would be related with the relaxation of the internal loops in the SCNPs as argued for the SCNPs in the bulk. This is the mechanism which determines the final relaxation at long times. In the nanocomposite, the displacements of SCNPs' hydrogens display enhanced deviations from Gaussian and exponential behavior compared with the pure melt of SCNPs. These effects would be due to the speed up of the motions of the SCNPs at short times induced by the surrounding faster linear precursor dynamics. On the other hand, the motions in the linear matrix are faster than in the bulk precursor material –an a priori unexpected result. These combined effects result in an averaged behavior that coincides with that of the pure precursor. This observation is in accordance with the macroscopic finding by DSC experiments – from which no impact of the presence of SCNPs on the material with respect to the pure matrix dynamics is deduced. This study demonstrates the power of QENS combined with isotopic labeling to selectively

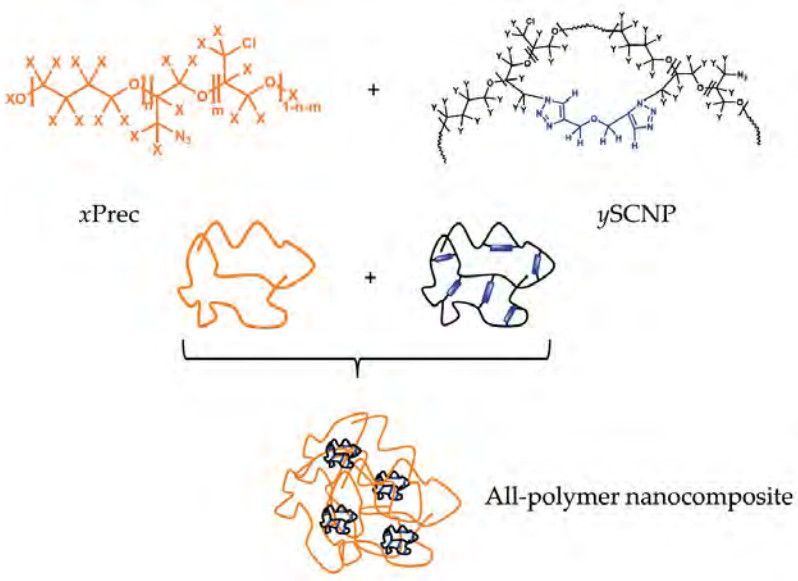


Figure 1: *Schematic illustration of all-polymer nanocomposite composition.*

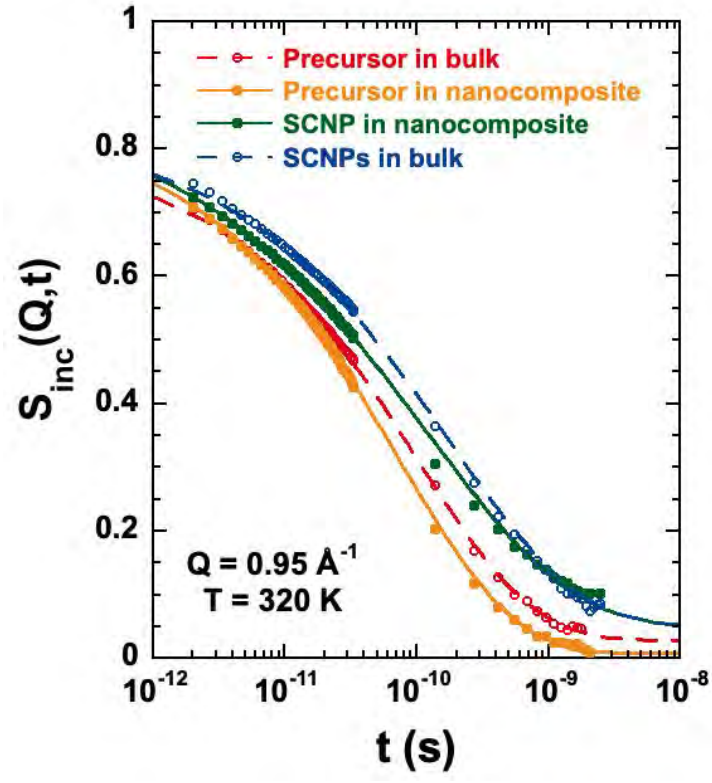


Figure 2: *Fourier-transformed and deconvoluted QENS spectra of the precursor and SCNPs in their respective bulk materials (empty circles) and as components in the nanocomposites (full squares).*

characterize component dynamics at microscopic level in complex materials like all-polymer nanocomposites, and resolve subtle effects that are overlooked by macroscopic non-selective methods.

This microscopic and selective insight reveals the crucial role of the relaxation of the internal loops of the SCNPs, that induces an increase with time of the dynamic heterogeneity in the nanocomposite.

HIGHLIGHT 16 – Polymers and Soft matter

Impact of temperature and architecture on the interfacial structure of microgels: a neutron reflectometry and computer simulations study

Steffen Bochenek, Fabrizio Camerin, Emanuela Zaccarelli, Armando Maestro, Maximilian M. Schmidt, Walter Richtering and Andrea Scotti.

Nature Communications 13, 3744 (2022)

This study provides an in-depth microscopic description of how different microgel architectures affect their arrangements at interfaces, and will be the foundation for a better understanding of their phase behavior and assembly. Both aspects are crucial to preparing smart emulsions that can be broken on demand.

Soft microgels—cross-linked polymer networks swollen in a good solvent—reveal peculiar properties that are different from those of other colloidal systems such as hard nanoparticles, polymers, and surfactants. Particularly, microgels based on poly-N-isopropylacrylamide (pNIPAM) have a high interfacial activity and at the same time maintain their thermo-responsiveness once adsorbed to air, liquid-, or solid interfaces.

The structural characterization of pNIPAM microgels at interfaces is fundamental to understand both their 2D phase behavior and their role as stabilizers that enable emulsions to be broken on demand as a function of external stimuli such as temperature and pH. However, this characterization is usually limited by available experimental techniques, which do not allow a direct investigation at interfaces.

To overcome this difficulty, the authors employ neutron reflectometry (NR), which allows them to probe the structure and responsiveness of the microgels in-situ at the air-water interface. Bochenek et al. investigate two types of microgels with different cross-link density, thus having different softness and deformability, both below and above their volume phase transition temperature, by combining NR experiments with computer simulations of in silico synthesized microgels. The advantage of NR is that it allows to probe the structure of a statistically significant ensemble of microgels in situ at the interface. Using NR, the authors can directly measure the protrusion of the microgels in the air and estimate how it changes with temperature.

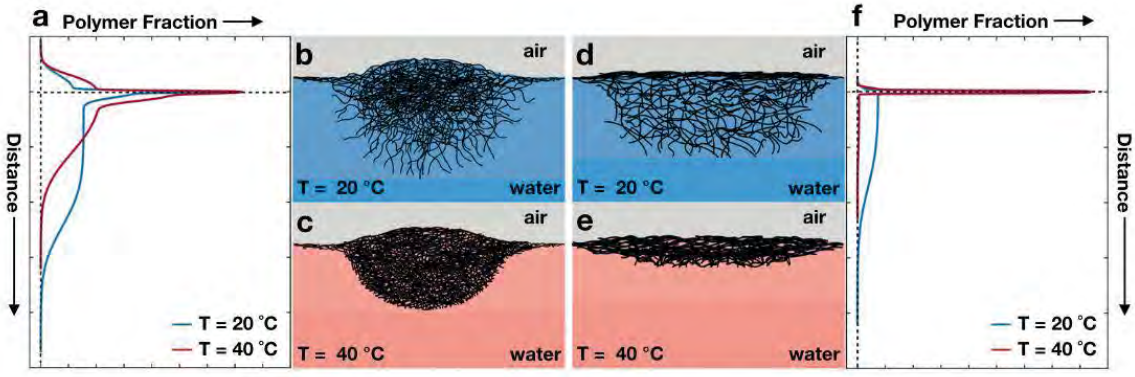


Figure: *Sketch of the adsorbed microgels. a The vertical profiles of standard microgels and f the vertical profiles of ULC microgels below and above the VPTT. Their corresponding shapes are outlined in b–e. The shapes are based on the combination of the team's polymer fraction profiles, simulations and AFM measurements at the liquid-solid interface from the literature.*

Microscopy-based techniques, such as transmission X-ray microscopy (TXM) or cryo-SEM, are usually limited by the small number of observed particles, the size of the particles, an observation direction perpendicular to the interface, and complicated sample preparation.

In this contribution, they found that temperature only affects the portion of microgels in water, while the strongest effect of the microgels softness is observed in their ability to protrude into the air. In particular, standard microgels have an apparent contact angle of few degrees, while ultra-low cross-linked microgels form a flat polymeric layer with zero contact angle.

The differences highlighted in the structure may be relevant for a more comprehensive understanding of microgels' effective interactions, paving the way for a better description of their 2D assembly and for a clever design of their applications such as emulsion stabilizers.

"This collaborative work bringing together scattering techniques and computer simulations is important to shed light on the collective behavior of microgels at interfaces."

HIGHLIGHT 17 – Quantum beams

Unraveling the ordered phase of the quintessential hybrid perovskite — thermophysics to the rescue

Pelayo Marin-Villa, Ana Arauzo, Kacper Drużbicki, and Félix Fernandez-Alonso.

The Journal of Physical Chemistry Letters 13, 8422 (2022) [ACS Editor´s Choice]

Hybrid (organic-inorganic) perovskites were discovered in the 1970s. Until quite recently, they were widely regarded as mere academic curiosities because of their rather exotic 'ionic-plastic-crystal' character. Today, they have become one of the most promising platforms for the development and subsequent deployment of next-generation photovoltaic and photonic technologies.

Notwithstanding the above, taming the stability of hybrid perovskites remains an unresolved challenge, deeply rooted in the complexity of their physico-chemical behaviour. The ongoing ´hybrid-perovskite fever´ in materials research is, therefore, in dire need of a robust microscopic picture of their multitude of phases, as well as of the nature and extent of the underlying disorder. In this work, Marin-Villa et al. have addressed this ongoing challenge for the case of the ordered phase of methylammonium lead iodide (MAPbI3), the most-celebrated hybrid perovskite. To this end, the authors have combined state-of-the-art neutron-scattering techniques, computational materials modelling and thermophysical data into a single and unified framework. At low temperatures, they find that the specific heat of $MAPbI_3$ exhibits strong and systematic deviations from the Debye limit, a common feature in pure hybrid perovskites and their mixtures. This analysis and interpretation of the experimental data using first-principles calculations shows that the local structure around the organic cation is characterized by a substantial lowering of the local symmetry relative to what is inferred from crystallographic (time-averaged) studies. Furthermore, the physical origin of the observed thermophysical anomalies can be explained quantitatively in terms of the presence of sub-Terahertz optical photons, associated with translational-librational distortions of the octahedral (inorganic) units. In the particular case of $MAPbI_3$, our results also make it evident that widely accepted structural models lead to overly strong interactions between the organic and inorganic sublattices.

These new insights have been possible by undertaking a detailed assessment of the performance of last-generation density functionals, via a direct comparison of their predictions with experimental data. The former have reached a sufficient level of maturity such that plausible structural models can now be scrutinized in unprecedented detail. Methodologically, we have made use of a hitherto unexploited experimental observable for quantitative model selection – the heat capacity. To the best of our knowledge, this is the first time that such a protocol has been implemented with success in hybrid perovskites, and anticipate that its realm of applicability can be extended to other classes of materials where other experimental probes fall quite short at providing physical insight.

"For the first time, state-of-the-art neutron scattering, first-principles calculations and thermophysical data are combined to unveil the structure of $MAPbI_3$."

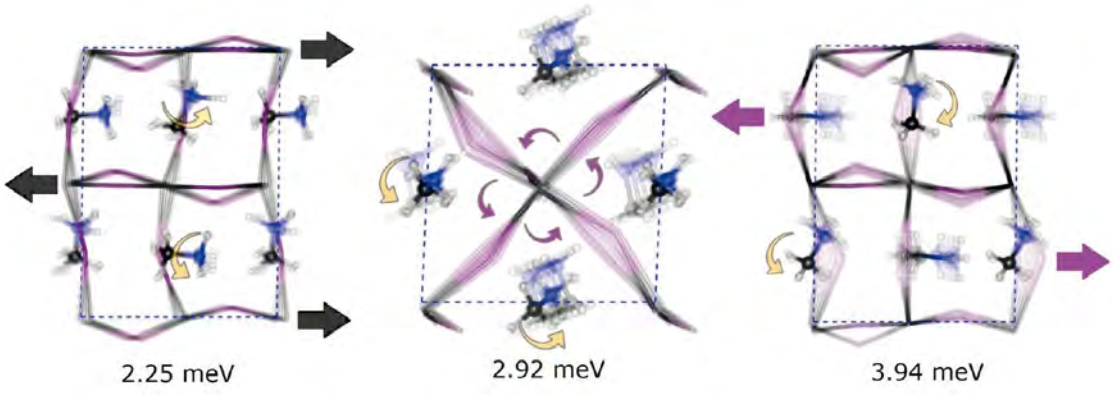


Figure: *Representative low-energy modes responsible for the thermophysical anomalies observed in $MAPbI_3$.*

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 building in 2010, state of the-art facilities have been launched progressively, which complete a set of very sophisticated and specialized experimental techniques, ready to give response to the needs in advanced materials characterization. These needs involve both generic research in nanomaterials, as well as specifically targeted systems of interest in energy and biological environments, perfectly aligned with the Smart Specialization Strategy (RIS3) and the 2030 Science, Technology and Innovation Plan (PCTI 2030) of the Basque Country, as well as with the IKUR Strategic lines defined by the Basque Department of Education.

FACILITIES

HIGHLIGHTED NEW EQUIPMENT

LIQUID HELIUM RECOVERY AND SUPPLY PLANT FOR CRYOGENIC EXPERIMENTAL SYSTEMS

In 2019, the CFM received funding from the Ministry of Science and Innovation, co-financed with Feder funds and CSIC funds, to acquire and install a helium gas recovery and liquefaction plant for the cryogenic experimental systems present at CFM, which has been successfully installed in 2022. 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 was compromised. The acquisition of a Helium recovery and supply plant has proven a permanent solution to this problem, also providing the CFM and its researchers with a common benefit facility that reduces research costs and cover a greater number of projects.

CHEMICAL PHYSICS OF COMPLEX MATERIALS

HIGH RESOLUTION ANGLE RESOLVED PHOTOEMISSION LAB

The "High Resolution Angle Resolved Photoemission" laboratory is equipped with an Angle Resolved Photoemission Spectroscopy (ARPES) system combined with atomic-resolved microscopy (Scanning Tunnel Microscope, STM). These two techniques can be used either jointly or separately. The ARPES instrument allows achieving ultra-high resolution (0.1 degrees, 5 meV) and can deal with samples at low temperature (40K). Samples can be prepared independently at two different preparation chambers and they can be inserted in the instrument via a fast-entry lock.

SURFACE CHEMICAL-PHYSICS LAB

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

SURFACE MAGNETISM LAB

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

ULTRA-LOW TEMPERATURE SCANNING TUNNELING MICROSCOPY LAB

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

FACILITIES

ELECTRONIC PROPERTIES AT THE NANOSCALE

CERAMICS AND CEMENT-BASED MATERIALS LAB

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

- High temperature ceramic ovens (Thermolyne model from ThermoFisher Scientific)
- A high temperature microwave oven that features 3100 Watts of microwave power and controllable temperature up to 2000°C (BP-211/50 model from Microwave Research and Applications, Inc.)
- Sub- and super-critical reactors (Novoclave 600ml HP 500bar/500°C)

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

PHOTONICS

LASER SPECTROSCOPY LAB

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

ULTRAFAST SPECTROSCOPY LAB

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

NANOPHOTONICS AND NANOMATERIALS SYNTHESIS LAB

The "Nanomaterials and Spectroscopy" group runs a laboratory for the synthesis of metallic and semiconducting nanoparticles, nanocrystals and nanocomposites, and another one for the characterization of their optical properties. The "Nanomaterials Synthesis Lab" is equipped with a fume hood, benches and state of the art equipment for colloidal synthesis, including a spin coater, centrifuges, thermocycler, thermostats, cryostat, high-precision programmable syringe and micropumps and balances. The "Nanophotonics" laboratory hosts a scanning confocal time-resolved photoluminescence microscopy setup (MicroTime200) with single-molecule detection sensitivity, equipped with two lasers (405 and 485 nm), two single-photon counting avalanche photodetectors, heating stage, and cryostat. The system contains the complete optics and electronics for recording all main aspects of the luminescence dynamics down to a single nanoparticle/molecule level with a wide range of capabilities: 2D and 3D confocal photoluminescence microscopy imaging, single-molecule imaging, 2D and 3D Fluorescence Lifetime Imaging (FLIM), the minor carrier's lifetime mapping, carrier's recombination dynamics, Resonance Energy Transfer (FRET).

Other available set-ups in these two labs include:

- QUEPRO high-performance spectrophotometer connected to IX71 Olympus microscope for micro-photoluminescence spectroscopy

FACILITIES

- 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).

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 nanopositioners, for cooling down nanostructures and nanoparticles to cryogenic temperatures (attoDRY 100 model from Attocube)
- A set of spatial light modulators (from Cambridge Correlators), polarizers (from Thorlabs and Standa) and Single Photon Counting Modules (SPCM, APDs SPCM-AQ4C model from Excelitas), for analyzing the photons interacting with nanostructures at cryogenic temperatures

FACILITIES

- Microwave generators and amplifiers (SMB100A model from Rohde & Schwartz), for addressing the electronic states of Nitrogen Vacancy centers in diamond

POLYMERS, SOFT MATTER & SUSTAINABLE MATERIALS P(SM)$_2$

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)

CHEMISTRY LAB

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

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

FACILITIES

THERMAL CHARACTERIZATION LAB

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

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

RHEOLOGICAL CHARACTERIZATION LAB

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

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

ABSORPTION SPECTROSCOPY TECHNIQUES LAB

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

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

X-RAY LAB

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

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

LIGHT SCATTERING LAB

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

HIGH PERFORMANCE COMPUTING (HPC) CENTRE

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

There are currently four CFM HPC clusters:

FACILITIES

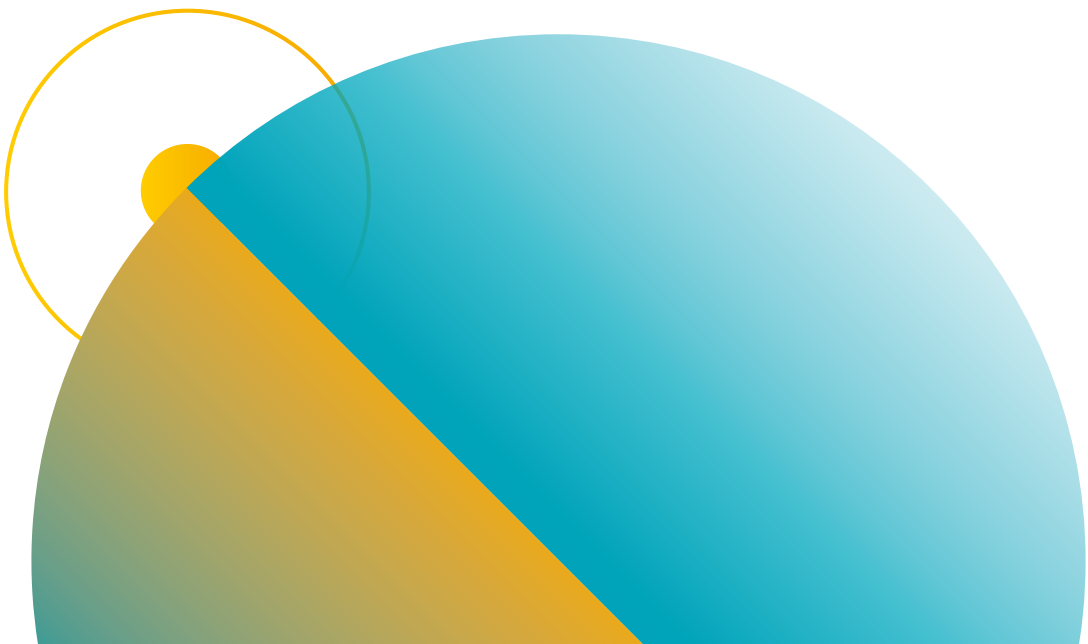
- Oberon cluster (the main, general purpose, CFM HPC cluster), composed of 182 computing nodes with two Xeon processors and a memory range of 24 GB up to 256 GB per node, all of them sharing a high speed-low latency Infiniband connection network and a high performance shared parallel filesystem, giving a total of 2000 cores and 15 TB of memory. This cluster gives service to the whole CFM research community.

- Nostromo cluster, targeted to shared memory – single node molecular dynamics calculations. It is composed of 17 AMD Opteron 6300 series computing nodes with 64 cores and 64 GB of RAM each node, giving a total of 1088 cores and about 1.1 TB of memory.

- Ekhi cluster, designed specifically for novel Quantum ESPRESSO calculations, is composed of 28 computing nodes with two Xeon Cascade Lake-SP 6230 processors (40 computing cores) and 96 GB of memory in each node, with an Infiniband FDR interconnection network, giving a total of 1120 cores and 2.7 TB of memory.

- Sama is a multipurpose cluster designed for high-level ab initio electronic structure calculations and molecular dynamics simulations. It is composed of 13 computing nodes with two Intel Xeon Gold 6240R processors (48 cores), 384 GB of memory, and 1 TB NVMe SSD disk per node, all interconnected through an Infiniband HDR 100 Gb/s network, and giving a total of 624 cores and 4.8TB of memory.

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



EXTERNAL SERVICES

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

ULTRA-LOW TEMPERATURE SCANNING TUNNELING MICROSCOPY

Hosts an Atomic Force Microscopy (AFM) / Scanning Tunnel Microscope (STM) operable at 1 K for characterisation of materials at atomic scale.

SURFACE MAGNETISM ANALYSIS

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

DIFFERENTIAL THERMAL ANALYSIS (DTA)

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

ISOBARIC THERMAL EXPANSION

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

ABSORPTION SPECTROSCOPY IN TERAHERTZ (THZ) DOMAIN

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

DIELECTRIC CHARACTERIZATION

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

SMALL-ANGLE X-RAY DIFFRACTION

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

MATERIALS SURFACE CHARACTERIZATION

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

NANOPHOTONICS LAB

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

HIGH PERFORMACE COMPUTING (HPC) SUPPORT

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

RESEARCH OUTPUT

At a glance

80%
Published in the Framework of International Collaborations

207
ISI Publications

Q1 WOS: **56%**

Q1 SCOPUS: **84%**

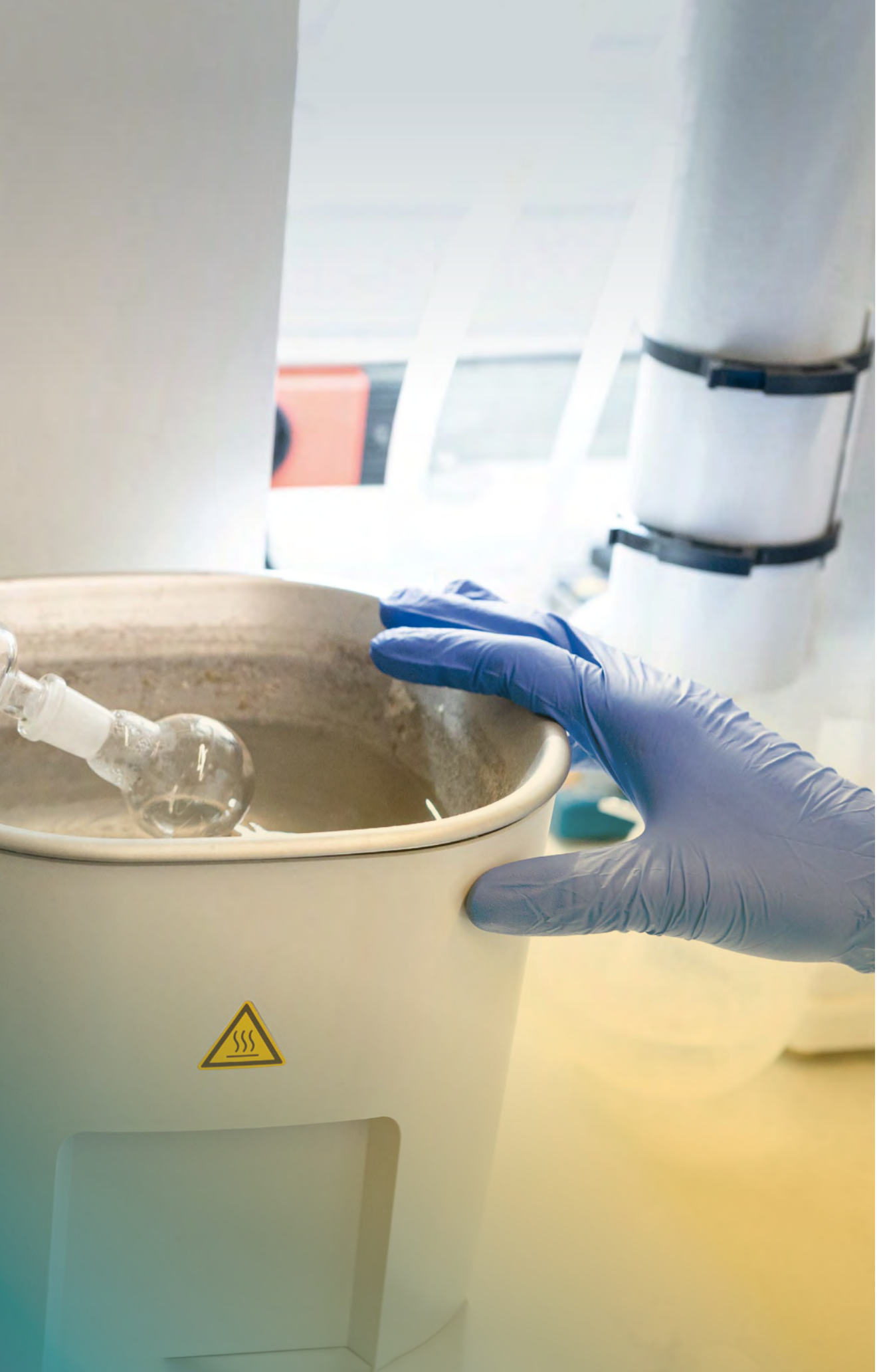
D1 WOS: **24%**

D1 SCOPUS: **39%**

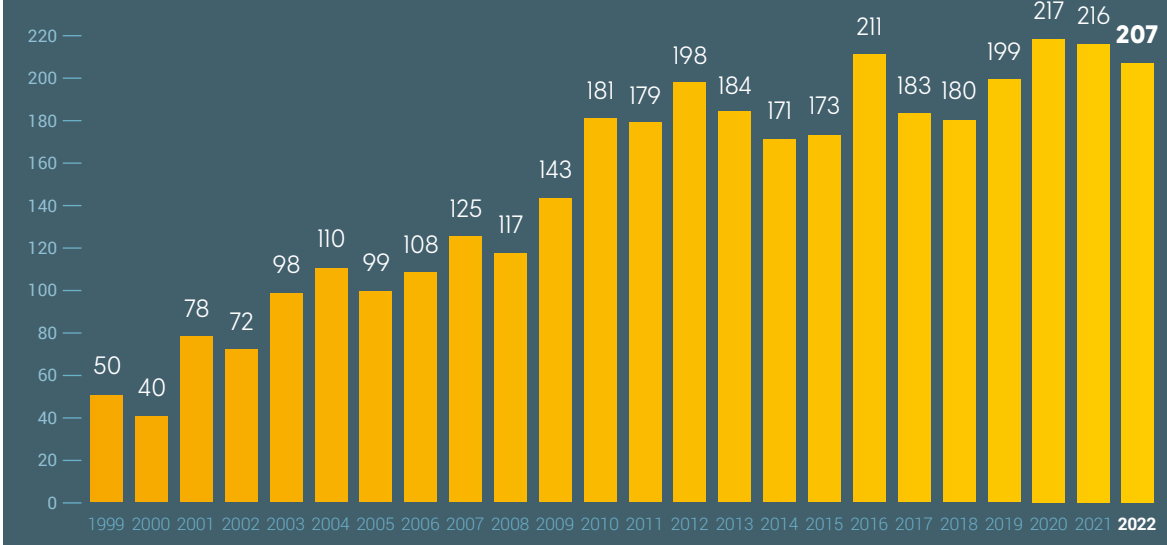
H-Index
150

ISI Web of Science citations
14 620* in 2022

*As of April 2023

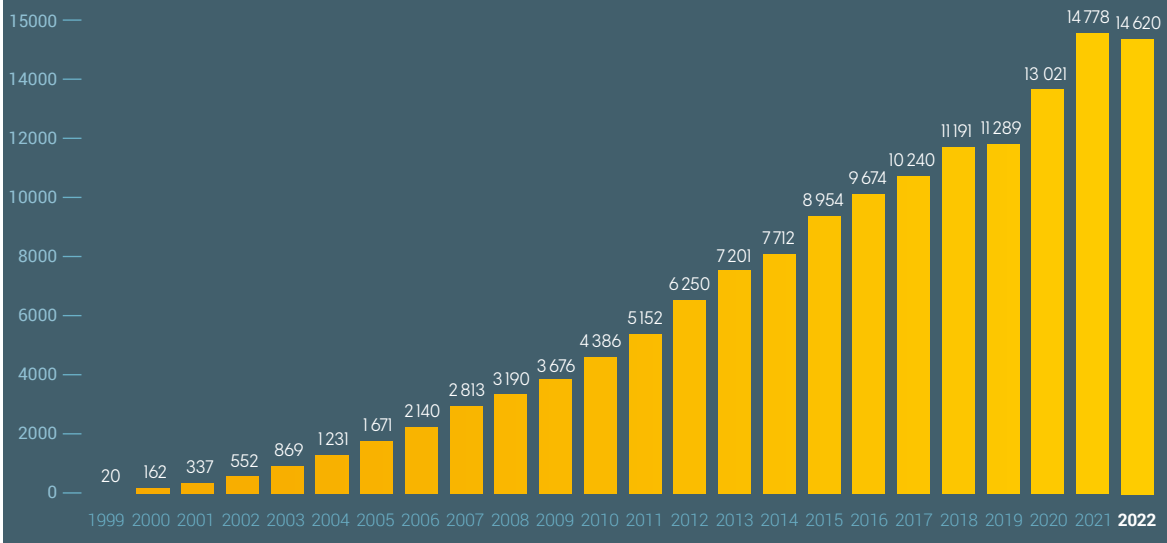


PUBLICATIONS



Evolution of the publications of CFM over the years.
Total number of ISI Publications since 1999 as of April 2023: 3539

CITATIONS



Evolution of the citations of CFM over the years.
Total number of citations since 1999 as of April 2023: 150 117

Total number of top publications*: 61

JOURNAL	N° OF ARTICLES	IMPACT FACTOR
Chemical Reviews	1	72,087
Nature	1	69,504
Reviews of Modern Physics	1	50,485
Nature Materials	1	47,656
Nature Reviews Physics	1	36,273
Advanced Materials	3	32,086
Progress in polymer Science	1	31,281
Accounts of Chemical Research	1	24,466
Nature Chemistry	1	24,274
Advanced Functional Materials	3	19,924
ACS Nano	5	18,027
Nature Communications	6	17,694
Advanced Science	1	17,521
Journal of the American Chemical Society	5	16,383
Materials Horizons	1	15,717
Advances in Colloid and Interface Science	1	15,190
Small	1	15,153
Physical Review X	1	14,417
Nano Letters	4	12,262
Cement and Concrete Research	1	11,958
ACS Applied Materials & Interfaces	3	10,383
Journal of Colloid and Interface Science	4	9,965
Physical Review Letters	5	9,185
Journal of Energy Storage	1	8,907
Nanoscale	4	8,307
Analytical Chemistry	1	8,008
Nanophotonics	1	7,923
Advanced Electronic Materials	1	7,633
ACS Photonics	1	7,08

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

PUBLICATIONS

1 **Molecular optomechanics approach to surface-enhanced Raman scattering**
Esteban R, Baumberg JJ, and Aizpurua J.
Accounts of Chemical Research 55, 1889 (2022)

2 **Spin hall magnetoresistance effect from a disordered interface**
Catalano S, Gomez-Perez JM, Aguilar-Pujol MX, Chuvilin A, Gobbi M, Hueso LE, and Casanova F.
ACS Applied Materials & Interfaces

3 **Intrinsic ferromagnetism in 2D Fe_2H with a high Curie temperature**
Ding SC, Yan X, Bergara A, Zhang XH, Liu Y, and Yang GC.
ACS Applied Materials & Interfaces 14, 44745 (2022)

4 **Hydrophobic gold nanoparticles with intrinsic chirality for the efficient fabrication of chiral plasmonic nanocomposites**
Kowalska N, Bandalewicz F, Kowalski J, Gomez-Grana S, Bagiriski M, Pastoriza-Santos I, Grzelczak M, Matraszek J, Perez-Juste J, and Lewandowski W.
ACS Applied Materials & Interfaces 14, 50013 (2022)

5 **Proximity effects on the charge density wave order and superconductivity in single-layer $NbSe_2$**
Dreher P, Wan W, Chikina A, Bianchi M, Guo HJ, Harsh R, Manas-Valero S, Coronado E, Martinez-Galera AJ, Hofmann P , Miwa JA, and Ugeda MM.
ACS Nano 15, 19430 (2022)

6 **Addressing electron spins embedded in metallic graphene nanoribbons**
Friedrich N, Menchon RE, Pozo I, Hieulle J, Vegliante A, Li JC, Sanchez-Portal D, Pena D, Garcia-Lekue A, and Pascual JI.
ACS Nano 16, 14819 (2022)

7 **Role of the magnetic anisotropy in atomic- spin sensing of 1 D molecular chains**
Wackerlin C, Cahlik A, Goikoetxea J, Stetsovych O, Medvedeva D, Redondo J, Svec M, Delley B, Ondracek M, Pinar A, Blanco-Rey M, Kolorenc J, Arnau A, and Jelinek P.
ACS Nano 16, 16402 (2022)

8 **Extracting pure circular dichroism from hierarchically structured CdS magic cluster films**
Yao Y, Ugras TJ, Meyer T, Dykes M, Wang D, Arbe A, Bals S, Kahr B, and Robinson RD.
ACS nano 16, 20457 (2022)

9 **Interlayer coupling of a two-dimensional kondo lattice with a ferromagnetic surface in the antiferromagnet $CeCo_2P_2$**
Poelchen G, Rusinov IP, Schulz S, Guttler M, Mende M, Generalov A, Usachov DY, Danzenbacher S, Hellwig J, Peters M, Kliemt K, Kucherenko Y, Antonov VN, Laubschat C, Chulkov EV, Ernst A, Kummer K, Krellner C, and Vyalikh DV.
ACS Nano 16, 3573 (2022)

10 **Suppressing platinum electrocatalyst degradation via a high-surface-area organic matrix support**
Smiljanic M, Bele M, Moriau LJ, Santa JFV, Menart S, Sala M, Hrnjic A, Jovanovic P, Ruiz-Zepeda F, Gaberscek M, and Hodnik N.
ACS Omega 7, 3540 (2022)

PUBLICATIONS

11 **Neat protein single-chain nanoparticles from partially denatured BSA**
de Molina PM, Le TP, Iturrospe A, Gasser U, Arbe A, Colmenero J, and Pomposo JA.
ACS Omega 7, 42163 (2022)

12 **Second-harmonic generation from a quantum emitter coupled to a metallic nanoantenna (Correction)**
Babaze A, Esteban R, Aizpurua J, and Borisov AG.
ACS Photonics 9, 1829 (2022)

13 **Decoupling of glassy dynamics from viscosity in thin supported poly(n-butyl methacrylate) films**
Chowdhury M, Monnier X, Cangialosi D, and Priestley RD.
ACS Polymers Au 2, 333 (2022)

14 **Strong Rashba effect and different f-d hybridization phenomena at the surface of the heavy-fermion superconductor $CeIrIn_5$**
Mende M, Ali K, Poelchen G, Schulz S, Mandic V, Tarasov AV, Polley C, Generalov A, Fedorov AV, Guttler M, Laubschat C, Kliemt K, Koroteev YM, Chulkov EV, Kummer K, Krellner C, Usachov DY, and Vyalikh DV.
Advanced Electronic Materials 8, 2100768 (2022)

15 **Designing artificial fluorescent proteins: squaraine-LmrR biophosphors for high performance deep-red biohybrid light-emitting diodes**
Ferrara S, Mejias SH, Liutkus M, Renno G, Stella F, Kociolek I, Fuenzalida-Werner JP, Barolo C, Coto PB, Cortajarena AL, and Costa RD.
Advanced Functional Materials 22, 2111381 (2022)

16 **Magnetic properties of layered hybrid organic-inorganic metal-halide perovskites: transition metal, organic cation and perovskite phase effects**
Asensio Y, Marras S, Spirito D, Gobbi M, Ipatov M, Casanova F, Mateo-Alonso A, Hueso LE, and Martin-Garcia B.
Advanced Functional Materials 32, 2207988 (2022)

17 **Percolating superconductivity in air-stable organic-ion intercalated MoS_2**
Pereira JM, Tezze D, Niehues I, Asensio Y, Yang HZ, Mester L, Chen S, Casanova F, Bittner AM, Ormaza M, Schiller F, Martin-Garcia B, Hillenbrand R, Hueso LE, and Gobbi M.
Advanced Functional Materials 32, 2208761 (2022)

18 **Exchange bias in molecule/Fe_3GeTe_2 van der Waals heterostructures via spinterface effects**
Jo J, Calavalle F, Martin-Garcia B, Tezze D, Casanova F, Chuvilin A, Hueso LE, and Gobbi M.
Advanced Materials 32, 2200474 (2022)

19 **Nontrivial doping evolution of electronic properties in ising-superconducting alloys**
Wan W, Wickramaratne D, Dreher P, Harsh R, Mazin II, and Ugeda MM.
Advanced Materials 34, 2200492 (2022)

20 **Observation of superconducting collective modes from competing pairing instabilities in single-layer $NbSe_2$**
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21 **Magnetic interplay between pi-electrons of open-shell porphyrins and d-electrons of their central transition metal ions**
Sun Q, Mateo LM, Robles R, Ruffieux P, Bottari G, Torres T, Fasel R, and Lorente N.
Advanced Science 9, 2105906 (2022)

22 **A broad perspective to particle-laden fluid interfaces systems: from chemically homogeneous particles to active colloids**
Guzman E, Martinez-Pedrero F, Calero C, Maestro A, Ortega F, and Rubio RG.
Advances in Colloid and Interface Science 302, 102620 (2022)

23 **Mapping the networked context of Copernicus, Michelangelo, and Della Mirandolla in wikipedia**
Miccio LA, Gamez-Perez C, Suarez JL, and Schwartz GA.
Advances in Complex Systems 25, 2240010 (2022)

24 **Separation, identification, and confirmation of cyclic and tadpole macromolecules via UPLC-MS/MS**
O'Neill JM, Mao JL, Haque FM, Barroso-Bujans F, Grayson SM, and Wesdemiotis C.
Analyst 147, 2089 (2022)

25 **Hydrogen detection limits and instrument sensitivity of high-resolution broadband neutron spectrometers**
Scatigno C, Zanetti M, Rudic S, Senesi R, Andreani C, Gorini G, and Fernandez-Alonso F.
Analytical Chemistry 94, 5023 (2022)

26 **Superconducting proximity effect in d-wave cuprate/graphene heterostructures**
Perconte D, Bercioux D, Dlubak B, Seneor P, Bergeret FS, and Villegas JE.
Annalen der Physik 534, 2100559 (2022)

27 **TMDs as a platform for spin liquid physics: A strong coupling study of twisted bilayer WSe_2**
Kiese D, He YC, Hickey C, Rubio A, and Kennes DM.
APL Materials 10, 031113 (2022)

28 **A patchy particle model for C-S-H formation**
Prabhu A, Dolado JS, Koenders EAB, Zarzuela R, Mosquera MJ, Garcia-Lodeiro I, and Blanco-Varela MT.
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29 **Polyelectrolyte/surfactant films: from 2D to 3D structural control**
Carrascosa-Tejedor J, Santamaria A, Tummino A, Varga I, Efstratiou M, Lawrence MJ, Maestro A, and Campbell RA.
Chemical Communications 58, 10687 (2022)

30 **Bio-inspired membranes for adsorption of arsenic via immobilized L-Cysteine in highly hydrophilic electrospun nanofibers**
Picon D, Torasso N, Baudrit JRV, Cerveny S, and Goyanes S.
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31 **O_2 on Ag(110): a puzzle for exchange-correlation functionals**
Loncaric I, Alducin M, and Juaristi JI.
Chemical Physics 554, 111424 (2022)

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32 **Cluster approach to scattering in MoS_2 photoemission**
Ambrosio MJ, Plesiat E, Decleva P, Echenique PM, Muino RD, and Martin F.
Chemical Physics 557, 111476 (2022)

33 **Absence of isotope effects in the photo-induced desorption of CO from saturated Pd(111) at high laser fluence**
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34 **Molecular approach to engineer two-dimensional devices for CMOS and beyond-CMOS applications**
Zhao YD, Gobbi M, Hueso LE, and Samori P.
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35 **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 (2022)

36 **Atomistic study of the effect of crystallographic orientation on the twinning and detwinning behavior of NiTi shape memory alloys**
Fazeli S, Izadifar M, Dolado JS, Ramazani A, and Sadrnezhaad SK.
Computational Materials Science 203, 111080 (2022)

37 **Spin reorientation in CoV_2O_4 thin film: A first principles study**
Sharma M, Krishna J, and Maitra T.
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38 **Along the road to crystal structure prediction (CSP) of pharmaceutical-like molecules**
Dudek MK, and Druzbicki K.
Crystengcomm 24, 1665 (2022)

39 **Special issue on broadband dielectric spectroscopy and its applications**
Napolitano SS, Wubbenhorst M, Schonhals A, and Cerveny S.
IEEE Transactions on Dielectrics and Electrical Insulation 29, 1221 (2022)

40 **Reactivity of $B(C_6F_5)_3$ towards glycidol: the formation of branched cyclic polyglycidol structures**
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Euopean Polymer Journal 171, 111194 (2022)

41 **$(PVDF)_2$ $(PEO)_2$ miktoarm star copolymers: synthesis and isothermal crystallization leading to exclusive beta-phase formation**
Maria N, Patil Y, Polymeropoulos G, Peshkov A, Rodionov V, Maiz J, Hadjichristidis N, and Muller AJ.
European Polymer Journal 179, 111506 (2022)

42 **Dilational rheology of fluid/fluid interfaces: foundations and tools**
Guzman E, Maestro A, Carbone C, Ortega F, and Rubio RG.
Fluids 7, 335 (2022)

43 **Editorial: biomimetic and bioinspired membranes to reconstruct the properties of natural systems**
Almendro Vedia VG, Martinez-Pedrero F, Maestro A, Guzman E, and Natale P.
Frontiers in Molecular mBiosciences 9, 1079570 (2022)

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44 **Structure and luminescent properties of Sm/Dy-doped $Sr_2MgSi_2O_7$ glass-ceramics**
Fernandez-Rodriguez L, Balda R, Fernandez J, Duran A, and Pascual MJ.
International Journal of Applied Glass Science 14, 140 (2022)

45 **Effect of the TrFE content on the crystallization and SSA thermal fractionation of P(VDF-co-TrFE) copolymers**
Maria N, Le Goupil F, Cavallo D, Maiz J, and Muller AJ.
International Journal of Molecular Sciences 23, 10365 (2022)

46 **Cementitious materials as promising radiative coolers for solar cells**
Cagnoni M, Tibaldi A, Dolado JS, and Cappelluti F.
iScience 25, 105320 (2022)

47 **Lattice dynamics of Bi_2Te_3 and vibrational modes in Raman scattering of topological insulators $MnBi_2Te_4$ center dot n(Bi_2Te_3)**
Abdullaev NA, Amiraslanov IR, Aliev ZS, Jahangirli ZA, Sklyadneva IY, Alizade EG, Aliyeva YN, Otrokov MM, Zverev VN, Mamedov NT, and Chulkov EV.
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48 **Dynamic stability of submonolayer structures in the Li/Cu(111) system**
Rusina GG, Borisova SD, and Chulkov EV.
JETP Letters 116, 261 (2022)

49 **Dehydroxylation processing and lasing properties of a Nd alumino-phosphate glass**
Munoz-Quinonero M, Azkargorta J, Iparraguirre I, Jimenez-Rioboo RJ, Tricot G, Shao CY, Munoz F, Fernandez J, and Balda R.
Journal of Alloys and Compounds 896, 163040 (2022)

50 **Zinc glycolate $Zn(OCH_2CH_2O)$: Synthesis and structure, spectral and optical properties, electronic structure and chemical bonding**
Krasil'nikov VN, Tyutyunnik AP, Zhukov VP, Baklanova IV, Gyrdasova OI, and Chulkov EV.
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Puppin M, Nicholson CW, Monney C, Deng Y, Xian RP, Feldl J, Dong S, Dominguez A, Hubener H, Rubio A, Wolf M, Rettig L, and Ernstorfer R.
Physical Review B 105, 075417 (2022)

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150 **Semilocal approximations to the Kohn-Sham exchange potential as applied to a metal surface**
Horowitz CM, Proetto CR, and Pitarke JM.
Physical Review B 105, 085149 (2022)

151 **Corner modes of the breathing kagome lattice: origin and robustness**
Herrera MAJ, Kempkes SN, de Paz MB, Garcia-Etxarri A, Swart I, Smith CM, and Bercioux D.
Physical Review B 105, 085411 (2022)

152 **Scattering effects from neighboring atoms in core-level WSe_2 photoemission**
Ambrosio MJ, Plesiat E, Decleva P, Echenique PM, Muino RD, and Martin F.
Physical Review B 105, 125405 (2022)

153 **Out-of-plane magnetic anisotropy in bulk ilmenite $CoTiO_3$**
Arruabarrena M, Leonardo A, Rodriguez-Vega M, Fiete GA, and Ayuela A.
Physical Review B 105, 144425 (2022)

154 **Quasiparticle density of states and triplet correlations in superconductor/ferromagnetic-insulator structures across a sharp domain wall**
Hijano A, Golovach VN, and Bergeret FS.
Physical Review B 105, 174507 (2022)

155 **Magnetic ordering and topology in $Mn_2Bi_2Te_5$ and $Mn_2Sb_2Te_5$ van der Waals materials**
Eremeev SV, Otrokov MM, Ernst A, and Chulkov EV.
Physical Review B 105, 195105 (2022)

156 **Nonlinear σ model for disordered systems with intrinsic spin-orbit coupling**
Virtanen P, Bergeret FS, and Tokatly IV.
Physical Review B 105, 224517 (2022)

157 **Yu-Shiba-Rusinov states in two-dimensional superconductors with arbitrary Fermi contours**
Ortuzar J, Trivini S, Alvarado M, Rouco M, Zaldivar J, Yeyati AL, Pascual JI, and Bergeret S.
Physical Review B 105, 245403 (2022)

158 **Enhanced superconductivity in CuH_2 monolayers**
Yan X, Ding SC, Zhang XH, Bergara A, Liu Y, Wang YC, Zhou XF, and Yang GC.
Physical Review B 106, 014514 (2022)

159 **Coupling the Higgs mode and ferromagnetic resonance in spin-split superconductors with Rashba spin-orbit coupling**
Lu Y, Ojajarvi R, Virtanen P, Silaev MA, and Heikkila TT.
Physical Review B 106, 024514 (2022)

160 **Multiplet effects in the electronic correlation of one-dimensional magnetic transition metal oxides on metals**
Goikoetxea J, Friedrich C, Bihlmayer G, Blugel S, Arnau A, and Blanco-Rey M.
Physical Review B 106, 035130 (2022)

161 **Directly probing the chirality of Majorana edge states**
Lu Y, Virtanen P, and Heikkila TT.
Physical Review B 106, 045139 (2022)

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162 **Nature of interfacial Dzyaloshinskii-Moriya interactions in graphene/Co/Pt(111) multilayer heterostructures**
Blanco-Rey M, Bihlmayer G, Arnau A, and Cerda JI.
Physical Review B 106, 064426 (2022)

163 **Three-dimensional Fermi surfaces from charge order in layered CsV_3Sb_5**
Huang XW, Guo CY, Putzke C, Gutierrez-Amigo M, Sun Y, Vergniory MG, Errea I, Chen D, Felser C, and Moll PJW
Physical Review B 106, 064510 (2022)

164 **Strain-induced collapse of Landau levels in real Weyl semimetals**
Lee YJ, Park CH, and Vozmediano MAH.
Physical Review B 106, 075125 (2022)

165 **Converging tetrahedron method calculations for the nondissipative parts of spectral functions**
Ghim M, and Park CH.
Physical Review B 106, 075126 (2022)

166 **Impact of ionic quantum fluctuations on the thermodynamic stability and superconductivity of $LaBH_8$**
Belli F, and Errea I.
Physical Review B 106, 134509 (2022)

167 **Structural and electronic properties of Na-B-H compounds at high pressure**
Li X, Zhang XH, Bergara A, Liu Y, and Yang GC.
Physical Review B 106, 174104 (2022)

168 **Crystal structure and Raman-active lattice vibrations of magnetic topological insulators $MnBi_2Te_4$? $n(Bi_2Te_3)$ (n=0, 1, ...,6)**
Amiraslanov IR, Aliev ZS, Askerova PA, Alizade EH, Aliyeva YN, Abdullayev NA, Jahangirli ZA, Otrokov MM, Mamedov NT, and Chulkov EV.
Physical Review B 106, 184108 (2022)

169 **Tunneling spectroscopy of few-monolayer $NbSe_2$ in high magnetic fields: Triplet superconductivity and Ising protection**
Kuzmanovic M, Dvir T, LeBoeuf D, Ilic S, Haim M, Mockli D, Kramer S, Khodas M, Houzet M, Meyer JS, Aprili M, Steinberg H, and Quay CHL.
Physical Review B 106, 184514 (2022)

170 **Towards comprehension of the surface state properties in the intrinsic magnetic topological insulators**
Men'shov VN, Shvets IA, and Chulkov EV.
Physical Review B 106, 205301 (2022)

171 **Field-free anomalous junction and superconducting diode effect in spin-split superconductor/topological insulator junctions**
Kokkeler TH, Golubov AA, and Bergeret FS.
Physical Review B 106, 214504 (2022)

172 **Absence of sizable superconductivity in hydrogen boride: a first-principles study**
Meninno A, and Errea I.
Physical Review B 106, 214508 (2022)

PUBLICATIONS

173 **Measurement of the Xe-136 two-neutrino double-beta-decay half-life via direct background subtraction in NEXT**
Novella P, Sorel M, Uson A, Adams C, Almazan H, Alvarez V, Aparicio B, Aranburu AI, Arazi L, Arnquist IJ, Ayet S, Azevedo CDR, Bailey K, Ballester F, Benlloch-Rodriguez JM, Borges FIGM, Bounasser S, Byrnes N, Carcel S, Carrion JV, Cebrian S, Church E, Conde CAN, Contreras T, Cossio FP, Denisenko AA, Diaz G, Diaz J, Dickel T, Escada J, Esteve R, Fahs A, Felkai R, Fernandes LMP, Ferrario P, Ferreira AL, Foss FW, Freitas EDC, Freixa Z, Generowicz J, Goldschmidt A, Gomez-Cadenas JJ, Gonzalez R, Gonzalez-Diaz D, Guenette R, Gutierrez RM, Haefner J, Hafidi K, Hauptman J, Henriques CAO, Morata JAH, Herrero-Gomez P, Herrero V, Ifergan Y, Jones BJP, Kekic M, Labarga L, Laing A, Larizgoitia L, Lebrun P, Gutierrez DL, Lopez-March N, Losada M, Mano RDP, Martin-Albo J, Martinez A, Martinez-Lema G, Martinez-Vara M, McDonald AD, Meziani ZE, Mistry K, Monrabal F, Monteiro CMB, Mora FJ, Vidal JM, Navarro K, Nygren DR, Oblak E, Odriozola-Gimeno M, Palmeiro B, Para A, Perez J, Querol M, Raymond A, Redwine AB, Renner J, Ripoll L, Rivilla I, Garcia YR, Rodriguez J, Rogero C, Rogers L, Romeo B, Romo-Luque C, Santos FP, dos Santos JMF, Simon A, Stanford C, Teixeira JMR, Thapa P, Toledo JF, Torrent J, Veloso JFCA, Vuong TT, Webb R, White JT, Woodruff K, and Yahlali N.
Physical Review C 105, 055501 (2022)

174 **Spin-polarizing electron beam splitter from crossed graphene nanoribbons**
Sanz S, Papior N, Giedke G, Sanchez-Portal D, Brandbyge M, and Frederiksen T.
Physical Review Letters 129, 037701 (2022)

175 **Simulating terahertz field-induced ferroelectricity in quantum paraelectric $SrTiO_3$**
Shin DB, Latini S, Schafer C, Sato SA, Baldini E, De Giovannini U, Hubener H, and Rubio A.
Physical Review Letters 129, 167401 (2022)

176 **Dynamics of two ferromagnetic insulators coupled by superconducting spin current**
Ojajarvi R, Bergeret FS, Silaev MA, and Heikkila TT.
Physical Review Letters 128, 167701 (2022)

177 **Theory of the supercurrent diode effect in rashba superconductors with arbitrary disorder**
Ilic S, and Bergeret FS.
Physical Review Letters 128, 177001 (2022)

178 **Dramatic plasmon response to the charge-density-wave gap development in 1T-$TiSe_2$**
Lin ZJ, Wang CX, Balassis A, Echeverry JP, Vasenko AS, Silkin VM, Chulkov EV, Shi YG, Zhang JD, Guo JD, and Zhu XT.
Physical Review Letters 129, 187601 (2022)

179 **Probing the role of grain boundaries in single Cu nanoparticle oxidation by in situ plasmonic scattering**
Nilsson S, Posada-Borbon A, Zapata-Herrera M, Fanta ABD, Albinsson D, Fritzsche J, Silkin VM, Aizpurua J, Gronbeck H, Esteban R, and Langhammer C.
Physical Review Materials 6, 045201 (2022)

180 **Effect of the valence state on the band magnetocrystalline anisotropy in two-dimensional rare-earth/noble-metal compounds**
Blanco-Rey M, Castrillo-Bodero R, Ali K, Gargiani P, Bertran F, Sheverdyaeva PM, Ortega JE, Fernandez L, and Schiller F.
Physical Review Research 4, 13237 (2022)

181 **Relaxation of photoexcited hot carriers beyond multitemperature models: general theory description verified by experiments on Pb/Si(111)**
Kratzer P, Rettig L, Sklyadneva IY, Chulkov EV, and Bovensiepen U.
Physical Review Research 4, 33218 (2022)

PUBLICATIONS

182 **Class of distorted Landau levels and Hall phases in a two-dimensional**
Sidler D, Rokaj V, Ruggenthaler M, and Rubio A.
Physical Review Research 4, 43059 (2022)

183 **Moire dispersion of edge states in spin chains on superconductors**
Mier C, Choi DJ, and Lorente N.
Physical Review Research 4, L032010 (2022)

184 **Mapping Lamb, Stark, and Purcell effects at a chromophore-picocavity junction with hyper-resolved fluorescence microscopy**
Roslawska A, Neuman T, Doppagne B, Borisov AG, Romeo M, Scheurer F, Aizpurua J, and Schull G.
Physical review X 12, 011012 (2022)

185 **Solvent-structured PEDOT:PSS surfaces: fabrication strategies and nanoscale properties**
Sanviti M, Mester L, Hillenbrand R, Alegria A, and Martinez-Tong D.
Polymer 246, 124723 (2022)

186 **Bio-based semi-crystalline PEF: temperature dependence of the constrained amorphous interphase and amorphous chain mobility in relation to crystallization**
Righetti MC, Vannini M, Celli A, Cangialosi D, and Marega C.
Polymer 247, 124771 (2022)

187 **Stars, combs and bottlebrushes of elastic single-chain nanoparticles**
Arena D, Verde-Sesto E, and Pomposo JA.
Polymer 258, 125315 (2022)

188 **Crystallization and phase separation in PEDOT:PSS/PEO blend thin films: influence on mechanical and electrical properties at the nanoscale**
Sanviti M, Martinez-Tong DE, Rebollar E, Ezquerra TA,and Garcia-Gutierrez MC.
Polymer 262, 125475 (2022)

189 **Comment on "Anomalous structural recovery in the near glass transition range in a polymer glass: data revisited in light of temperature variability in vacuum oven-based experiments**
Cangialosi D, Alegria A, and Colmenero J.
Polymer Engineering and Science 62, 2716 (2022)

190 **Soft colloidal particles at fluid interfaces**
Guzman E, and Maestro A.
Polymers 14, 1133 (2022)

191 **Approaching polymer dynamics combining artificial neural networks and elastically collective nonlinear langevin equation**
Miccio LA, Borredon C, Casado U, Phan AD, and Schwartz GA.
Polymers 14, 1573 (2022)

192 **Macrocyclic polymers: Synthesis, purification, properties and applications**
Ochs J, Pagnacco CA, and Barroso-Bujans F.
Progress in polymer Science 134, 101606 (2022)

193 **Engineering quantum states and electronic landscapes through surface molecular nanoarchitectures**
Piquero-Zulaica I, Lobo-Checa J, Abd El-Fattah ZM, Ortega JE, Klappenberger F, Auwarter W, and Barth JV.
Reviews of Modern Physics 94, 045008 (2022)

PUBLICATIONS

194 **A method to estimate the size of single-chain nanoparticles under severe crowding conditions**
Asenjo-Sanz I, Verde-Sesto E, and Pomposo JA.
RSC Advances 12, 1571 (2022)

195 **Portable magnetic resonance imaging of patients indoors, outdoors and at home**
Guallart-Naval T, Algarin JM, Pellicer-Guridi R, Galve F, Vives-Gilabert Y, Bosch R, Pallas E, Gonzalez JM, Rigla JP, Martinez P, Lloris FJ, Borreguero J, Marcos-Perucho A, Negnevitsky V, Marti-Bonmati L, Rios A, Benlloch JM, and Alonso J.
Scientific Reports 12, 13147 (2022)

196 **Electron microscopy and calorimetry of proteins in supercooled water**
Melillo JH, Nikulina E, Iriarte-Alonso MA, Cerveny S, and Bittner AM.
Scientific Reports 12, 16512 (2022)

197 **Localization versus delocalization of *d*-states within the Ni_2MnGa Heusler alloy**
Janovec J, Zeleny M, Heczko O, and Ayuela A.
Scientific Reports 12, 20577 (2022)

198 **Assessing the role of interatomic position matrix elements in tight-binding calculations of optical properties**
Ibanez-Ibanez J, de Juan F, and Souza I.
Scipost Physics 12, 70 (2022)

199 **On the separation of Hall and ohmic nonlinear responses**
Tsirkin SS, and Souza I.
Scipost Physics Core 5, 039 (2022)

200 **Correlating symmetries of low-frequency vibrations and self-trapped excitons in layered perovskites for light emission with different colors**
Lin ML, Dhanabalan B, Biffi G, Leng YC, Kutkan S, Arciniegas MP, Tan PH, and Krahne R.
Small 18, 2106759 (2022)

201 **Fabrication and nanoscale properties of PEDOT:PSS conducting polymer nanospheres**
Sanviti M, Alegria A, and Martinez-Tong DE.
Soft Matter 18, 4554 (2022)

202 **Physical aging of hydroxypropyl methylcellulose acetate succinate via enthalpy recovery**
Seo Y, Zuo B, Cangialosi D, and Priestley RD.
Soft Matter 18, 8331 (2022)

203 **Geopolymer concrete performance study for high-temperature Thermal Energy Storage (TES) applications**
Rahjoo M, Goracci G, Martauz P, Rojas E , and Dolado JS.
Sustainability 14, 1937 (2022)

204 **Synthetic micro/nanomotors for drug delivery**
Guzman E, and Maestro A.
Technologies 10, 96 (2022)

205 **High throughput optimization procedure to characterize vitrification kinetics**
Abate AA, Cangialosi D, and Napolitano S.
Thermochimica Acta 707, 179084 (2022)

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206 **Thermodynamic analysis of dehydration of K_2CO_3.1.5H_2O**
Mazur N, Huinink H, Borm B, Sansota S, Fischer H, and Adan O.
Thermochimica Acta 715, 179286 (2022)

207 **Transport and optical properties of the chiral semiconductor Ag_3AuSe_2**
Won J, Kim S, Gutierrez-Amigo M, Bettler S, Lee B, Son J, Noh TW, Errea I, Vergniory MG, Abbamonte P, Mahmood F, and Shoemaker DP.
Zeitschrift fur Anorganische und Allgmeine Chemie 648, e202200055 (2022)

BOOK CHAPTERS

Shape-sensitive inelastic scattering from metallic nanoparticles

Apell SP, Mukhopadhyay G, Antosiewicz TJ, and Aizpurua J.

Advances in Quantum Chemistry 85, 17 (2022)

Glass Transition and Relaxation Phenomena

Cangialosi D.

Thermal Analysis of Polymeric Materials Methods and Developments 1, 227 (2022)

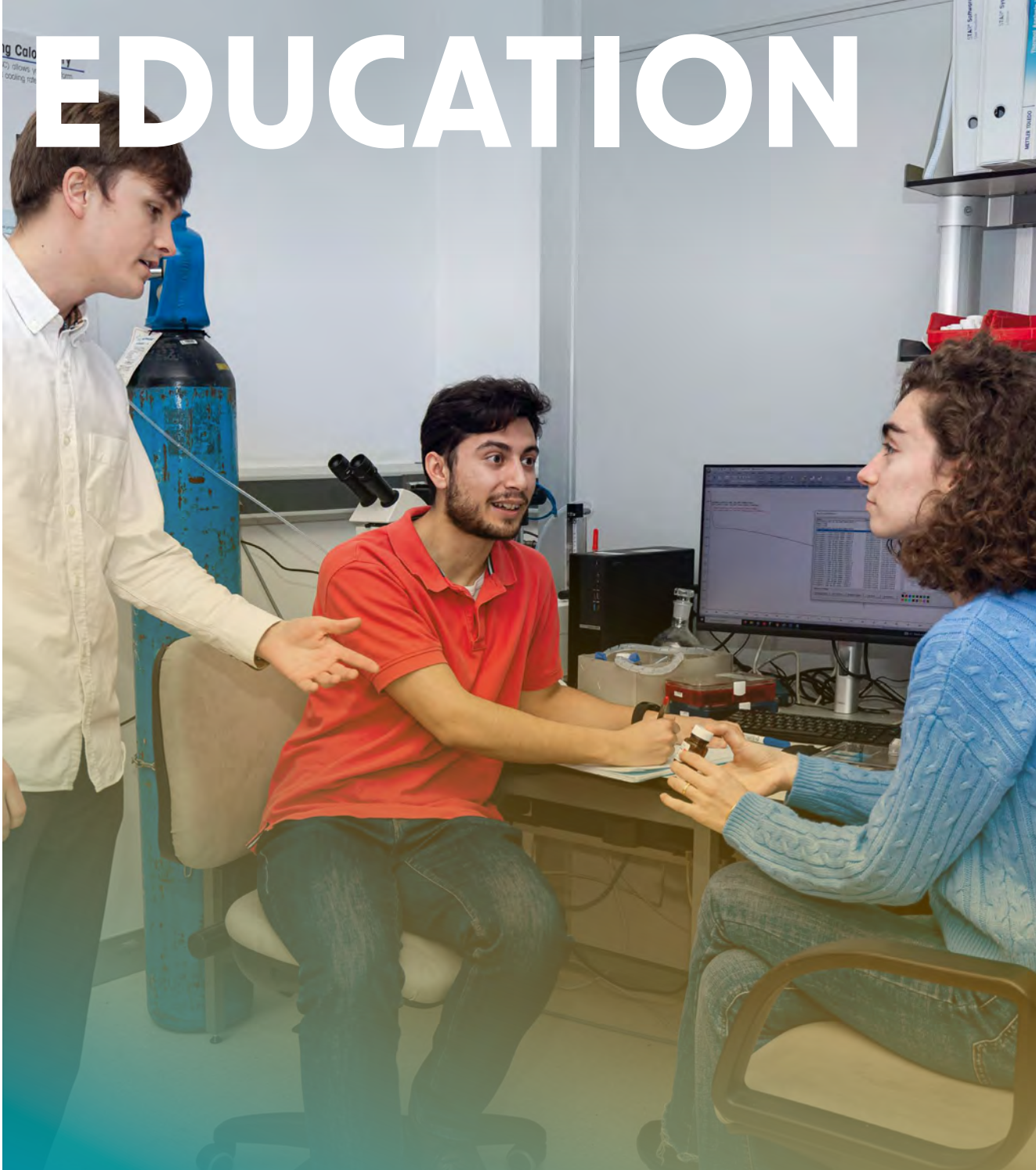
PATENTS APPLIED FOR

Composition for removing pharmaceuticals and heavy metals
22383090
Javier Martínez Sabando, Silvina Cerveny Murcia, Francesco Coin, Gustavo A. Schwartz Pomeraniec.

Low temperature production of synthetic wollastonite
PCT/EP22/076691
Jorge Sánchez Dolado.

Method for colorimetric detection of bacteria in food samples
21739369
María Jesús Grilló Dolset, Victoria Eugenia Garrido González, Javier Aizpurua Iriazabal, and Marek Grzelczak.

EDUCATION



As a joint center which belongs to the University of the Basque Country (UPV/EHU), the training activity at CFM includes the participation in both the Master and PhD program through the Department of Material Physics of UPV/EHU, as well as setting complementary training activities, and post-doctoral researchers training. All these activities are strongly related and coordinated with the research activity at the different research groups at CFM. In the following we note the main aspects of the training activities at CFM.

POST-DOCTORAL TRAINING

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

PHD PROGRAM: PHYSICS OF NANOSTRUCTURES AND ADVANCED MATERIALS

"Physics of Nanostructures and Advanced Materials" is a PhD program of UPV/EHU that has been recognized as a highly qualified PhD program by the Spanish Ministry of Education (MEE2011-0591 citation of excellence). Within this program, 70 PhD students develop their research fully embedded in the daily life of the research groups in the center.

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

DEFENDED PHD THESES

- **Heterogeneous catalysis on curved crystals: CO oxidation on Pt and Rh**
  Author: Fernando García Martínez
  Supervisor: Enrique Ortega Conejero and Frederik M. Schiller
  Group: Nanophysics Lab
  17/02/2022

- **Collective electronic and magnetic states in two-dimensional transition metal dichalcogenides**
  Author: Paul Dreher
  Supervisors: Miguel Moreno Ugeda
  Group: Miguel Moreno Ugeda´s group (DIPC)
  25/03/2022

- **Surface models of influenza virus envelope: biophysical studies under various hydration scenarios**
  Author: Maiara Aime Iriarte Alonso
  Supervisors: Alexander Bittner and Silvina Cerveny Murcia
  Group: Polymers and Soft Matter
  01/04/2022

- **Influence of the molecular topology on polymeric properties: a computational study of collapse, effective interactions and gelation**
  Author: Mariarita Paciolla
  Supervisor: Angel J. Moreno Segurado
  Group: Polymers and Soft Matter
  16/05/2022

- **Electronic correlation and magnetic properties of one-dimensional chains**
  Author: Joseba Goikoetxea Perez
  Supervisors: Andrés Arnau Pino and María Blanco Rey
  Group: Modelisation and simulation
  30/06/2022

- **Ab initio many-body perturbation theory to study molecular systems: from implementation to applications**
  Author: Masoud Mansouri
  Supervisors: Daniel Sánchez Portal and Peter Koval
  Group: Modelisation and simulation s
  04/10/2022

- **Quantum many-body effects in the optoelectronic response of plasmonic nanostructures and their coupling to quantum emitters**
  Author: Antton Babaze Aizpurua
  Supervisors: Ruben Esteban Llorente and Javier Aizpurua Iriazabal
  Group: Theory of nanophotonics
  04/11/2022

- **Non-enzymatic photoregeneration of cofactor molecules**
  Author: Karolina Kinastowska
  Supervisors: Wojciech Bartkowiak and Marek Grzelczak
  Group: Wroclaw University of Science and Technology and Nanomaterials and Spectroscopy (CFM)
  25/11/2022

- **Characterization of hydrogen based superconductors from first principles**
  Author: Francesco Belli
  Supervisors: Ion Errea Lope
  Group: Quantum theory of materials
  16/12/2022

SHORT STAYS IN FOREIGN UNIVERSITIES

A very important aspect of the PhD training program consists of supporting short stays in foreign universities and centers for PhD students. This year 5 pre-doctoral researchers have spent about 2-3 months in some of the best international centers on their topics. This training activity combines aspects of internationalization and excellence, and has been strongly supported within the last years by CFM. The following pre-doctoral researchers benefited from an internship abroad supported by CFM in 2022:

- **Matteo Sanviti**
  Universite libre de Bruxelles (ULB) (Brussels, Belgium)
  01-04/2022

- **Martín Gutierrez Amigo**
  Max Planck Institute (Dresden, Germany)
  01-06/2022

- **Alvaro Nodar Villa**
  Macquire University (Sydney, Australia)
  04-06/2022

- **Jon Lasa Alonso**
  Center of Theoretical Physics of the Polish Academy of Sciences (Warszawa, Poland)
  05-06/2022

- **Jokin Pinacho Olaciregui**
  LCPO- Organic Polymer Chemistry Laboratory, Université de Bordeaux (Brussels, Belgium)
  05-07/2022

- **Miriam Martínez Flórez**
  Wright Laboratory at Yale University (New Haven, USA)
  09-11/2022

- **Pelayo Marín Villa**
  Institut Laue-Langevin (Grenoble, France)
  09-11/2022

- **Alberto Hijano Mendizabal**
  The Institute of Nanoscience - CNR (Pisa, Italy)
  10-11/2022

- **Bruno Candelas Peñalba**
  Computational Electronic Structure Theory-Aalto University (Helsinki, Finland)
  11-12/2022

PHD RECRUITMENT FAIR 2022

In 2022 CFM organized the fifth PhD Recruitment Fair as part of the strategic plan to recruit new talent. From the 175 applications received, 20 applicants were shortlisted for online interviews. In the interviews, the candidates had the opportunity to discuss the research projects with the supervisors of the different projects and/or the Evaluation Committee.

After the evaluation, 4 candidates were selected and granted full studentships to join one research group at CFM:

- **Vasiliki Maria Stavropoulou**
  Group: Polymers and Soft Matter
  Supervisor: Daniele Cangialosi

- **Isabel Pascual Robledo**
  Group: Theory of nanophotonics
  Supervisor: Javier Aizpurua Iriazabal

- **Xabier Arrieta Aristi**
  Group: Theory of nanophotonics
  Supervisor: Rubén Esteban Llorente

- **Samuel Kerschbaumer**
  Group: Nanophysics lab
  Supervisor: Celia Rogero Blanco

MASTER EDUCATION PROGRAM

MASTER IN NANOSCIENCE

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

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

SCHOLARSHIPS

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

In 2022, three graduates were awarded scholarships for the Master in Nanoscience program:

- **Martin Irizar Landa**
  Supervisor: Aran Garcia-Lekue (DIPC)

- **Edurne Saenz Parraga**
  Supervisors: Aitzol García-Etxarri (DIPC) and Nuno de Sousa (DIPC)

- **Lorea Sanchez Fernández de Larrea**
  Supervisors: Santiago Blanco Canosa (DIPC)

- **Joseba Solozabal Aldalur**
  Supervisor: Gabriel Molina Terriza

THESES OF THE NANOSCIENCE MASTER SUCCESSFULLY DEFENDED IN 2022

- **Synthesis of protein based single chain nanoparticles and their characterization with scattering techniques**
  Author: David Gutierrez Armayor
  Supervisor: Paula Malo De Molina and Arantxa Arbe Méndez

- **Looking for the spin swapping effect**
  Author: Jone Mencos Frechila
  Supervisor: Felix Casanova (CIC nanoGUNE)

- **The effect of magnetic impurities on mutliple-Andreev reflections**
  Author: Parmenio Boronat
  Supervisors: Nicolás Lorente and Deung-Jang Choi

- **Computational design of magnetic 2D graphene nanoarchitectures**
  Author: Martin Irizar Landa
  Supervisors: Aran Garcia-Lekue (DIPC)

- **Cyclic poly(ethylene glycol) as nanoparticle surface ligand: physisorption vs. chemisorption**
  Author: June Aguirre Tolosa
  Supervisors: Fabienne Barroso Bujans (DIPC-CFM) and Marek Grzelczak

- **Machine learning applied to nanophotonics**
  Author: Edurne Saenz Parraga
  Supervisors: Aitzol García-Etxarri (DIPC) and Nuno de Sousa (DIPC)

- **Electronic friction between two graphene layers**
  Author: Nuria Santervas Arranz
  Supervisors: Emilio Artacho (CIC nanoGUNE) and Natalia Koval

- **Coupling reversible clustering of gold nanoparticles with chemo-thermal reaction**
  Author: Aimar Marauri Iriberri
  Supervisors: Marek Grzelczak

- **Novel carbon-based media for thermal energy storage applications - Phase behaviour and metastability**
  Author: Cristina Maciá Castello
  Supervisors: Félix Fernández Alonso

- **Electronic structure of CaCo2As2 studied using angle-resolved-photoemission spectroscopy and theoretical calculations**
  Author: Lorea Sanchez Fernández de Larrea
  Supervisors: Santiago Blanco Canosa

- **Theory of infrared electromagnetic near field in anisotropic layered materials as probed by realistic s-SNOM tips**
  Author: Isabel Pascual Robledo
  Supervisors: Javier Aizpurua Iriazabal

- **Synthesis of single chain nanoparticles of enzymes**
  Author: Pablo Ruiz Bozal
  Supervisors: Jose A. Pomposo Alonso and Paula Malo De Molina

- **Synthesis and Characterization of Precursors Towards Single Chain Nanoparticles for Energy Applications**
  Author: Manuel Gómez Menéndez
  Supervisors: Jose A. Pomposo Alonso and Jon Maiz Sancho

OTHER MASTER THESES PROJECTS SUPERVISED BY CFM STAFF AND SUCCESSFULLY DEFENDED IN 2022

- **Towards modeling the kondo effect for magnetic impurities in graphene: one and two-impurities Anderson model**
  Author: Daniel García Pina
  Supervisors: Daniel Sánchez Portal and Aran Garcia Lekue

- **Pares de Lewis frustrados para la polimerización por apertura de anillo de epóxidos**
  Author: Eric Gómez Urreizti
  Supervisor: Fabienne Barroso Bujans

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 **12** undergraduate students. CFM also offers the possibility to receive support for this training through different grant programs.

DEFENDED GRADE PROJECT

- **Exploration of the thermophysical properties of novel carbon-based materials**
  Author: Margherita Simoni
  Supervisor: Felix Fernandez

SCHOLARSHIP

- **Iñaki Fernández Tena**
  Supervisors: Martina Corso and Jose Ignacio Pascual (CIC nanoGUNE)
  Ikasiker from the Basque Government

WORKSHOPS, CONFERENCES, SEMINARS & COURSES

CFM scientists have organized or co-organized several international workshops and conferences during 2022. 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 dramatically the impact and relevance of the individual and groups' research outcome.

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Moreover, CFM researchers attended requests to give more than **70 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 2022 is as follows:

CONFERENCES

QENS/WINS 2022 - Conference on Quasielastic Neutron Scattering and Workshop on Inelastic Neutron Spectrometers

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

Miramar Palace (Donostia / San Sebastián)

23-27/05/2022

Current challenges in materials for thermal energy storage

organizers: Fernando Bresme (Imperial College London), and Felix Fernandez-Alonso (CFM).

Cecam (Lausanne, Switzerland)

8-10/06/2022

II International conference on Novel 2D materials explored via scanning probe microscopy & spectroscopy

Organizers: Miguel Moreno Ugeda (DIPC, CFM) and Iván Brihuega (IFIMAC / UAM).

Miramar Palace (Donostia / San Sebastián)

20-24/06/2022

International Meeting on Challenges and Opportunities for HICANS

Organizers: Senentxu Lanceros-Méndez (BCMaterials), Raquel González (BCMaterials), Mario Pérez (ESS Bilbao), Esfania Abad (ESS Bilbao), Juan Colmenero (CFM), Arantxa Arbe (CFM), and Erik Fernández (Ineustar).

BCMaterials (Leioa)

20-22/06/2022

QUANTUMatter 2022 - International conference on science and technology of quantum matter

Organizers: Antonio Correia (Phantoms Foundation) - Chairperson, Ricardo Díez Muiño (DIPC, CFM), Juan Jose Garcia-Ripoll (IFF), and Pablo Ordejon (ICN2).

AXA Convention Center (Barcelona)

21-23/06/2022

Quantum designer physics (QDP2022)

Organizers: Daniel Loss (University of Basel), Francisco Guinea (IMDEA Nanoscience, DIPC, Ikerbasque), Andres Arnau (CFM, DIPC) and Vitaly Golovach (CFM, DIPC, Ikerbasque).

Miramar Palace (Donostia / San Sebastián)

18-21/07/2022

11th conference on Broadband Dielectric Spectroscopy and its applications

Organizers: Silvina Cerveny (Chair person, CFM), Gustavo Ariel Schwartz (CFM), Daniele Cangialosi (CFM), Silvia Arrese-Igor (CFM), Claudia Borredon (CFM), Francesco Coin (CFM), Javier Martínez Sabando (CFM), and Jorge H. Melillo (CFM).

Cámara de Comercio (Donostia / San Sebastián)

4-9/09/2022

WOKSHOPS

Sustainable materials for energy storage solutions

Organizer: Jorge S. Dolado (CFM).

CFM

22-25/02/2022

1st MIRACLE workshop

Organizer: Jorge S. Dolado (CFM).

CFM

4-6/05/2022

LTC Green concrete industry open day

Organizer: Jorge S. Dolado (CFM).

CFM

22/06/2022

Photo and electrocatalysis at athe atomic scale

Organizers: Sara Barja (CFM), Celia Rogero (CFM), Ethan Crumlin (Lawrence Berkeley National Laboratoy, USA), and Martin Sterrer (University of Graz, Austria).

Miramar Palace (Donostia / San Sebastián)

22-23/06/2022

NeIC CodeRefinery workshop

Organizers: Nordic e-Infrastructure Collaboration (NeIC) - Local coordinators: Iñigo Aldazabal (CFM), and Abel Carreras (DIPC).

Online

22-24 and 29-30/06/2022

1st IKUR neutrionics workshop

Organizers: Daniel Sánchez Portal (CFM).

CFM

29/09/2022

On-surface synthesis international workshop (OSS22)

Organizers: Martina Corso (CFM), Dimas G. de Oteyza (DIPC, Ikerbasque), and André Gourdon (CEMES-CNRS).

Sant Feliu de Guixols (Girona)

25-30/09/2022

Membrane technologies for the treatment and recovery of water resources

Organizers: Silvina Cerveny (CFM), Silvia Goyanes (Universidad de Buenos Aires and CONICET, Argentina), and Jose Vega Baudrit (LANOTEC, Costa Rica).

CFM

10-11/10/2022

Transborder QuantumChemPhys Lab Workshop

Organizers: Pascal Larregaray (Université de Bordeaux, France) and Ricardo Díez Muiño (DIPC, CFM).

Hotel Le Bayonne (France)

13-14/10/2022

Artificial Intelligence for applied research. Practical approach

Organizers: Isabel Perez (Nemix), and Iñigo Aldazabal (CFM).

CFM

14/12/2022

Net zero carbon buildings | Energy neutral and sustainability in construction and building materials

organizers: Antonio Caggiano (UniGE) and Jorge S. Dolado (CFM).

Università degli Studi di Genova (Italy)

15/12/2022

COURSES

Photo and electrocatalysis at athe atomic scale

Organizers: Sara Barja (CFM), Celia Rogero (CFM), Ethan Crumlin (Lawrence Berkeley National Laboratoy, USA), and Martin Sterrer (University of Graz, Austria).

CFM

20-21/06/2022

The taming of energy

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

Miramar Palace (Donostia / San Sebastián)

4-6/07/2022

8th International doctoral training session: frontiers of condensed matter

organizers: Juan Ignacio Pérez Iglesias (UPV/EHU) and Ricardo Díez Muiño (DIPC, CFM).

Miramar Palace (Donostia / San Sebastián)

4-6/07/2022

RILEM Multi-scale Modelling Course for Concrete (MMC2)

Organizers: Erik Schlangen (Chair, TU Delft), Ye Guang (TU Delft), Branko Savija (TU Delft), Eddy Koenders (TU Darmstadt), Jorge S. Dolado (CFM).

TU Delft (The Netherlands)

3-7/10/2022

QUANTUM BREAKFAST

Starting in 2021, and promoted by CFM researcher Miguel Varga, "The Quantum Breakfast seminar series" intended to be educational in a distended atmosphere. They are a great opportunity to gain insight in quantum technologies, as well as to bring together the local community. In 2022, starting in April, they were organized on a monthly bases with three or four researchers sharing their experience and knowledge in each session.

APRIL 29	MAY 27	JUNE 25
Mikel Abadia Project Manager at DIPC, IKUR Quantum Technologies **Gabriel Molina-Terriza** Quantum Nanophotonics Laboratory – CFM **Nacho Pascual** Nanoimaging Laboratory – nanoGUNE **Pedro Crespo** Mathematical Foundations – TECNUN	**Josu Etxezarreta** Mathematical Foundations Group, Tecnun **Maxim Ilin** Nanophysics Laboratory, CFM **Roberto Álvarez** Molecular Electronic Structure group, DIPC.	**Patricio Fuentes Ugartemendia** Mathematical Foundations Group, Tecnun. **Rubén Pellicer** Quantum Nanophotonics Laboratory, CFM
SEPTEMBER 30	**OCTOBER 28**	**NOVEMBER 25**
David Novoa Department of Communications Engineering, School of Engineering (Bilbao) **Stefan Ilic** Mesoscopic Physics Group, CFM **Álvaro Nodar-Villa** Theory of Nanophotonics Group, CFM	**Adrián Juan Delgado** Theory of Nanophotonics group, CFM **Rubén Pellicer** Quantum Nanophotonics Laboratory, CFM **Antonio de Martí** Department of Biomedical Engineering and Sciences (IBC), Tecnun - School of Engineering of the University of Navarra	**Victor Krivenkov** Nanomaterials and Spectroscopy Group, CFM **Vitaly Golovach** Electronic Excitations in Surfaces and Nanostructures Group, CFM

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, media training or transformative leaderships. Around 80 researchers joined these courses in 2022.

Scientific writing basics

DIPC

4-6/04/2022

Speakers: Sofia Facal (Skills for Science and Industry).

The ability to present scientific findings and information in a written format is an essential skill for everyone that wishes to pursue a career in science. Unlike other types of writing, scientific writing follows a specific format and style.

This workshop on scientific writing skills provides an outline of this format for a research paper, shines light on the publication and peer review process and gives basic tips for communicating complex topics in a logical, clear and understandable way.

The content of the workshop included:

- Scientific authorship and good scientific practice
- Scientific journals and the peer review system
- Scientific Paper Structure: objective, key content and length of the sections
- Find your story: Development of the central idea
- How to choose and organize the content
- Handling raw data in publications
- Images and graphics
- The logical flow: Coherence and Cohesion
- Do's and Don'ts of paper writing

Seminar: mental health issues and the ethics of care in research intensive institutions

DIPC

24/05/2022

In this seminar Dr. Erin Huner, Director of Culture & Inclusion, at the Ivey Business School, discussed approaches to designing curricular and co-curricular learning opportunities for students that center equity, inclusion and well-being, as a means of increasing student success and sense of belonging within the post-secondary landscape.

Dr. Erin Huner - Faculty member and Director of Culture & Inclusion at the Ivey Business School

Dr. Erin Huner is an adjunct Faculty member and Director of Culture & Inclusion at the Ivey Business School. She is a social geographer with expertise in implementing research into practice in the areas of Equity Diversity and Inclusion and Gender Based Violence, Student Skill Acquisition and Student Mental Health and Wellbeing within the Post-Secondary sector.

Creatividad. El método Murakami

DIPC

1,8,15 and 22/06/2022

Speaker: Juan Luis Suárez, Director of CulturePlex Lab (Western University en Ontario, Canadá).

The different elements of the Murakami Method were studied in the light of similar ideas contributed by scientists (Poincaré), mathematicians (Whitehead), writers (Poe, Proust, Trollope), artists (Doris Salcedo, Theaster Gates), musicians (Seiji Ozawa), and chefs (Ferrán Adriá and Andoni Luis Aduriz). The classes were organised around the following themes:

- Illuminations
- Training
- Craftsmanship
- Originality

Emotional intelligence at work

CFM

30/11/2022 and 01/12/2022

Speaker: Sofia Facal (Skills for Science and Industry).

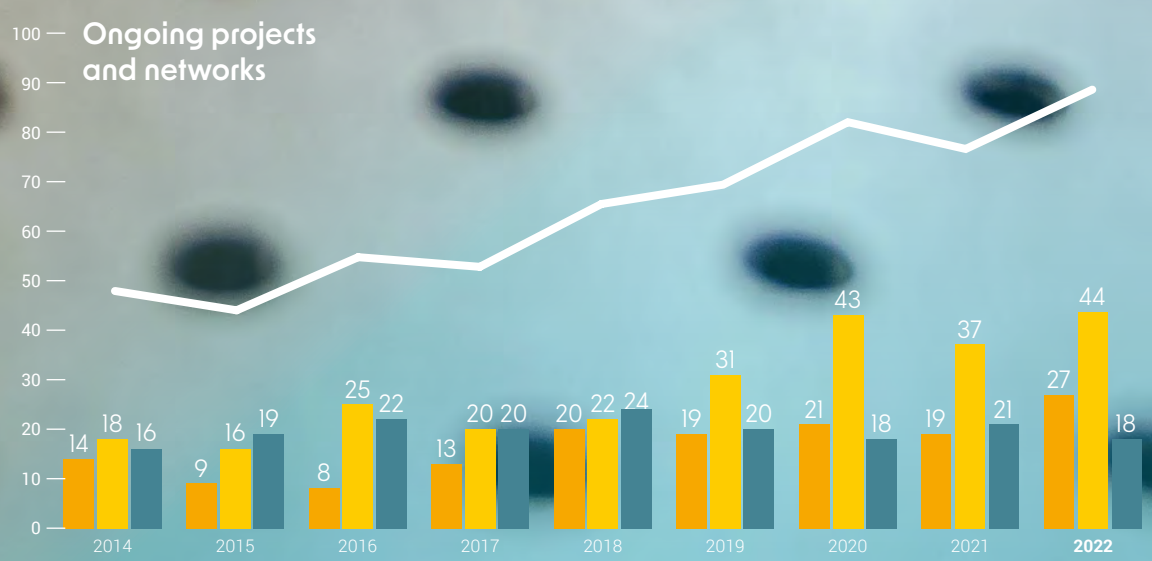
Our social skills and emotional intelligence competencies are enriching factors in the workplace and our daily life. However, despite their importance, most individuals aren't aware of these tools and how to develop them. This training focused on the fundamentals of emotional intelligence and the understanding of how it plays a role in our interpersonal relationships at work. The specialists Sofia Facal and Manuela Bercioux applied effective methods to enrich ourselves and the diverse world of academia.

The content of the workshop included:

- The basics of Emotional Intelligence
- Empathy and social skills: proficiency in managing relationships and building network
- Building Emotional Intelligence of Groups
- Emotional Intelligence and Diversity model: your cultural software
- The art of influence
- Collaboration and handling conflicts in the workplace

COMPETITIVE FUNDING FOR RESEARCH PROJECTS

RESEARCH PROJECTS AND NETWORKS	Competitive public fundraising in 2022
BASQUE	2 966 851.29 €
SPANISH MINISTRY	3 031 241.90 €
INTERNATIONAL	927 599.20 €
MPC-BERC	1 400 291.00 €
Total	8 325 983.39 €



The projects and networks ongoing during 2022 (a total of 89 projects/networks) are listed below according to the source of competitive funding.

BASQUE RESEARCH PROJECTS AND NETWORKS

- **EJ/GV, 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, 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, IKERTALDE 2022, Grupo Consolidado IT1569-22**

  Grupo de Fisicoquímica de Superficies y Nanoestructuras.

  PI: Iñaki Juaristi Oliden

- **EJ/GV, 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, 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, IKERTALDE 2022, Grupo Consolidado IT1453-22**

  FunThEMaS: Fundamental Theoretical and Experimental Materials Science.

  Partner: Lucia Vitali

BASQUE RESEARCH PROJECTS AND NETWORKS

- **EJ/GV, 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, Partidas directas 2022 – Tecnologías Cuánticas**

  Laboratorio de tecnologías cuánticas

  PI: Gabriel Molina Terriza

- **EJ/GV, Proyectos de Investigación Básica y/o Aplicada 2021-2023 (PIBA), PIBA2021_1_0026**

  Propiedades estructurales y electrónicas de perovskitas híbridas en condiciones variables de presión, temperatura, interfaces e iluminación

  PI: Lucia Vitali

- **EJ/GV, Proyectos de Investigación Básica y/o Aplicada 2020-2022 (PIBA), PIBA2020_1_0017**

  Hacia la computación cuántica topológica manipulando átomos en superconductores

  PI: Deungjang Choi

- **EJ/GV, Ayudas en el ejercicio 2022 para la adquisición de equipamiento científico, Ekizien 2022, EC_2022_1_0019**

  Calorimetro rapido de barrido de última generación

  PI: Felix Fernández

- **EJ/GV, Ayudas para la organización de congresos y reuniones de carácter científico, IKERBILERAK 2022, RC_2022_1_0005**

  QENS Conferences and WINS Conferences

  PI: Arantxa Arbe Mendez

- **EJ/GV, PREDOC BERRI 2020-21 y renovaciones**

  Balthasar Braunewell (year 1), Josu Diego López (year 2), Martín Gutiérrez Amigo (year 3)

BASQUE RESEARCH PROJECTS AND NETWORKS

- **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 2022, 2022-FELL-000009-01**

  Descripción teórica de reacciones térmicas en superficies.

  Beneficiary: Ane Escobar Fernández

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

  Desarrollo y fabricacion de los cirquitos electricos hibridos 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, 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, Deung-jang Choi

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2021-RED2021, Mod. Equipamiento, 2021-CIEN-000032-01**

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

  PI: Lucia Vitali

BASQUE RESEARCH PROJECTS AND NETWORKS

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

  Luz y diamantes: computación cuántica en Donostia

  PI: Gabriel Molina Terriza

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

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

  PI: Josetxo Pomposo Alonso

- **Fomento San Sebatián – 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

- **EusCampus Fundazioa, Fortalecimiento del LTC Green Concrete, el refuerzo de su conexión con la eurorregión.**

  PI: Jorge S. Dolado

- **UPV/EHU, proyectos estratégicos 2022, (PES22/84)**

  TOPO: theoretical and computational studies of the electronic properties of solids

  PI: Ivo S. Souza

- **UPV/EHU, proyectos estratégicos 2022, (PES21/32)**

  MagicFACE: Magnetic Hybrid Metal-Organic Interface

  PI: Enrique Ortega

- **UPV/EHU, Infrastructura 2022, (INF22/05)**

  Detector de dispersion de luz multiangulo de funcionamiento dual

  PIs: Angel Alegría Loinaz and Josetxo Pomposo Alonso

- **UPV/EHU, EHUko Sailentzako Laguntzak/Ayudas Departamentos UPV 2020, DEP20/61**

  Polímeros y materiales avanzados: física, química y tecnología

  PI: Iñaki Juaristi Oliden

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

  pI: Angel Moreno Segurado
  Co-PI: Josetxo Pomposo Alonso

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

  MAMI: Moleculas como Impurezas Magneticas para tecnologias cuánticas

  PI: Deungjang Choi
  Co-PI: 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: Teoria ab initio de respuestas de transporte y opticas de orden superior en cristales

  PI: Ivo Souza
  Co-PI: 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 límpias: nuevas estrategias físico-químicas (MACMAT)

  PI: Félix Fernándes Alonso y Pedro Braño 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)

  PI: Jon Mais Sancho y 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)

  PI: Jorge Sánchez Dolado y 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)

  PI: Celia Rogero Blanco y 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, degradadation 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

  PI: Sebastián Bergeret Sbarbaro

  Co-PI: Vitaly Golovach

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

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

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

  PI: Rolindes Balda de la Cruz

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

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

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

  PI: Sara Barja Martínez

  Co-PI: Frederik Michael Schiller

- **Acciones de Dinamización Europa Excelencia 2020, EUR2020-112116**

  ## ARTS - Atomic research for topological superconductors / Investigación atómica para superconductores topológicos

  PI: Deungjang Choi

- **Acciones de Dinamización Europa Excelencia 2020, EUR2020-112066**

  ## ReversO_2 - Oxygen conversion reactions: Fundamental insights for rational design

  PI: Sara Barja Martínez

- **Adquisición equipamiento Científico-Técnico 2019, Ministerio de Ciencia e Innovación, EQC2019-005735-P. Fondos Feder y CSIC central.**

  ## Instalación de una planta de recuperación y suministro de Helio líquido para sistemas experimentales criogénicos

  PI: Martina Corso

SPANISH RESEARCH PROJECTS AND NETWORKS

- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-104650GB-C21**

  ## Dinámica en soluciones acuosas de polímeros y biopolímeros (subproyecto coordinador)

  Proyecto Coordinado: BRIDGE - Cerrando la brecha entre los polímeros sintéticos y los biopolímeros - propiedades físicas y químicas

  PI: Silvina Cerveny Murcia

  Co-PI: Gustavo A. Schwartz Pomeraniec

- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-107396GB-I00**

  ## GASOLIN - Interfaces gas/sólido: acoplamiento entre la dinámica nuclear y la dinámica electrónica

  PI: Maite Alducin Ochoa

  Co-PI: Ricardo Díez Muiño

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

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

  PI: Andrés Ayuela Fernández

  Co-PI: Silkin Vyacheslav (DIPC, Ikerbasque)

- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-107432GB-I00**

  ## QUATOPHOT - Estudio de los efectos cuánticos en nanofotónica a escala atómica

  PI: Javier Aizpurua Iriazabal

  Co-PI: Rubén Esteban Llorente

- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-103910GB-I00**

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

  PI: Andrés Arnau Pino

  Co-PI: Asier Eiguren Goyenechea (UPV/EHU)

SPANISH RESEARCH PROJECTS AND NETWORKS

- **Proyectos de I+D+i de Retos Investigación 2019 (RTI2019), PID2019-111772RB-I00**

  ## QUATH - Análisis cuantitativo de la contribución de cargas calientes y efecto térmico en fotocatálisis asistida por efecto plasmónico

  PI: Marek Grzelczak

  Co-PI: Jon Mattin Matxain Beraza (UPV/EHU)

- **Proyectos de I+D+i de Retos Investigación 2019 (RTI2019), PID2019-107338RB-C63**

  ## FunMolSys - síntesis en superficie de sistemas moleculares funcionales (subproyecto)

  Proyecto Coordinado: MONOMET - Transferencia de sistemas moleculares funcionales a superficies no metálicas

  PI: Martina Corso

  Co-PI: Dimas García de Oteyza Feldermann (DIPC, Ikerbasque)

- **Proyectos de I+D+i de Retos Investigación 2019 (RTI2019), PID2019-107338RB-C66**

  ## TheoFunMolSys - Teoría de propiedades electrónicas, topológicas, magnéticas y vibracionales de nanoSistemas Moleculares Funcionales (subproyecto)

  Proyecto Coordinado: MONOMET - Transferencia de sistemas moleculares funcionales a superficies no metálicas

  PI: Daniel Sánchez Portal

  Co-PI: Arantzazu García Lekue (DIPC, Ikerbasque)

- **Proyectos de I+D+i Programación Conjunta Internacional 2019 (PCI2019-103657)**

  ## Functional porous cementitious nanocomposites for heat storage in buildings using phase materials

  PI: Jorge Sanchez Dolado

- **Adquisición de Equipamiento Científico-Técnico 2019, EQC2019-005735-P**

  ## Installation of a liquid Helium recovery and supply plant for cryogenic experimental systems

  PI: Martina Corso

- **Proyectos de I+D+i Retos Investigación 2018 (RTI2018), RTI2018-097895-B-C44**

  ## FUN-SOC - Novel functionalities driven by spin-orbit interactions

  PI: Nicolás Lorente Palacios

  Co-PI: Deungjang Choi

SPANISH RESEARCH PROJECTS AND NETWORKS

- **Proyectos de I+D+i Retos Investigación 2018 (RTI2018), RTI2018-098554-B-I00**

  E-CRETE - Energy storage solutions based on ConCRETE

  PI: Jorge Sánchez Dolado
  Co-PI: Juan José Gaitero Redondo (Tecnalia)

- **Redes Investigación 2018 - Red Temática, RED2018-102459-T**

  CAT&SCALE - (Photo-)Electrocatalysis: from the atomic scale to advanced devices

  pI, Network Coordinator: Sara Barja Martínez

- **Contratos Juan de la Cierva (JdC) 2021 FJC2021-047090-I**

  Chiral anapoles / Fuentes quirales no radiantes

  PI: Gabriel Molina Terriza
  Beneficiary: Jorge Olmos Trigo

- **Contratos Juan de la Cierva (JdC) 2021, FJC2021-047710-I**

  Non-equlibrium self-assembly and catalysis with metal nanoparticles

  PI: Marek Grzelczak
  Beneficiary: Anish Roa

- **Contratos Ramón y Cajal (RyC) 2017, RYC-2017-21931**

  Novel physical phenomena in two-dimensional materials

  PI: Sara Barja Martínez

- **Contratos Personal Técnico de Apoyo (PTA) 2021, PTA2021-020084-I**

  Apoyo técnico al laboratorio del grupo Ceramic and Cement-based Materials para el desarrollo the Photonic Metaconcrete y Thermoelectric Concrete del CFM - Centro Mixto CSIC-UPV/EHU

  Lab Technician: Guido Goracci
  Supervisor: Jorge Sanchez Dolado

- **Contratos Personal Técnico de Apoyo (PTA) 2019, PTA2019-018134-I**

  Apoyo técnico de los laboratorios de ultra-alto vacío del Centro de Física de Materiales (CFM)-Centro Mixto CSIC-UPV/EHU

  Lab Technician: Laura Fernández Gómez-Recuero
  Supervisor: Martina Corso

SPANISH RESEARCH PROJECTS AND NETWORKS

- **Contratos Personal Técnico de Apoyo (PTA) 2017, PTA2017-14359-I**

  Técnico para el laboratorio de rayos X del CFM (CSIC-UPV/EHU): mantenimiento del servicio y explotación de nuevas oportunidades de los equipos

  Lab Technician: Amaia Iturrospe Ibarra
  Supervisor: Arantxa Arbe Méndez

- **CSIC, Ayudas incorporación CSIC**

  Diseño de materiales cuánticos mediante moléculas magnéticas depositadas

  PI: Roberto Robbles Rodriguez

- **CSIC, I-LINK+2021, Colaboración Científica Internacional, LINKA20407**

  Hybrid nanomaterials for neuronal photostimulation

  PI: Marek Grzelczak

- **CSIC, I-COOP+ 2020, Cooperación Científica para el Desarrollo, COOPB20502**

  Arsenic-free, new nano-structured multifunctional materials to remove arsenic in groundwater

  PI: Silvina Cerveny Murcia

- **CSIC, I-LINK+2019, Colaboración Científica Internacional, LINKC20002**

  On-surface polymerization for high performance (opto)electronics

  PI: Martina Corso

- **CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2021, 2021AEP039**

  Novel functionalities driven by spin-orbit interaction (RTI2018-097895-B-C44)

  PI: Nicolás Lorente Palacios

- **CSIC, Fondo de Apoyo a los Servicios Científico Técnicos (FAS) 2022, FAS2022_005**

  Bomba turbomolecular - accesorio equipa existente

- **CSIC, Programa de Apoyo a la Infraestructura (PAI) 2022-2023, PAI2022_4026**

  Adecuación de laboratorios de ciencia de superficies del CFM

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

- **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

- **MSCA Doctoral Networks (HORIZON-MSCA-2021-DN-01), GA 101072964**

  QLUSTER: quantum and classical ultrasoft matter

  PI: Angel Moreno Segurado

- **HORIZON EUROPE Pathfinder Open (HORIZON-EIC-2021-PATHFINDEROPEN-01-01)**

  ESiM: Energy Storage in Molecules

  PI: Nicolas Lorente Palacios

- **ONR Global basic and applied scientific research grant (N62909-22-1-2031)**

  Microspherical superlens windows to the quantum world

  PI: Yury Rakovich

- **ERC Synergy Grant (ERC-2020-SyG), GA 951281**

  BOLD - A background-free experiment to discover the nature of neutrinos based on single Barium Atom Light Detection

  PI: Celia Rogero Blanco

- **ERC Starting Grant (ERC-2020-StG), GA 946629**

  PhotoNow - Discovery and Characterization of Third-Generation Nonlinear Photovoltaics

  PI: Julen Ibañez Azpiroz

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

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

  PI: Ion Errea Lope

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

- **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

- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020-FETOPEN-01-2018-2019-2020), GA 829067**

  THOR - TeraHertz detection enabled by mOleculaR optomechanics

  PI: Javier Aizpurua Iriazabal

- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020-FETOPEN-01-2016-2017), GA800923**

  SUPERTED - Thermoelectric detector based on superconductor-ferromagnet heterostructures

  PI: Sebastián Bergeret Sbarbaro

  Co-PI: Celia Rogero Blanco

- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020-FETOPEN-01-2016-2017), GA 766864**

  MEMO-Mechanics with Molecules

  PI: Nicolás Lorente Palacios

EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

- **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

- **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

- **COST Action 2017, CA17139**

  EUTOPIA - European Topology Interdisciplinary Action

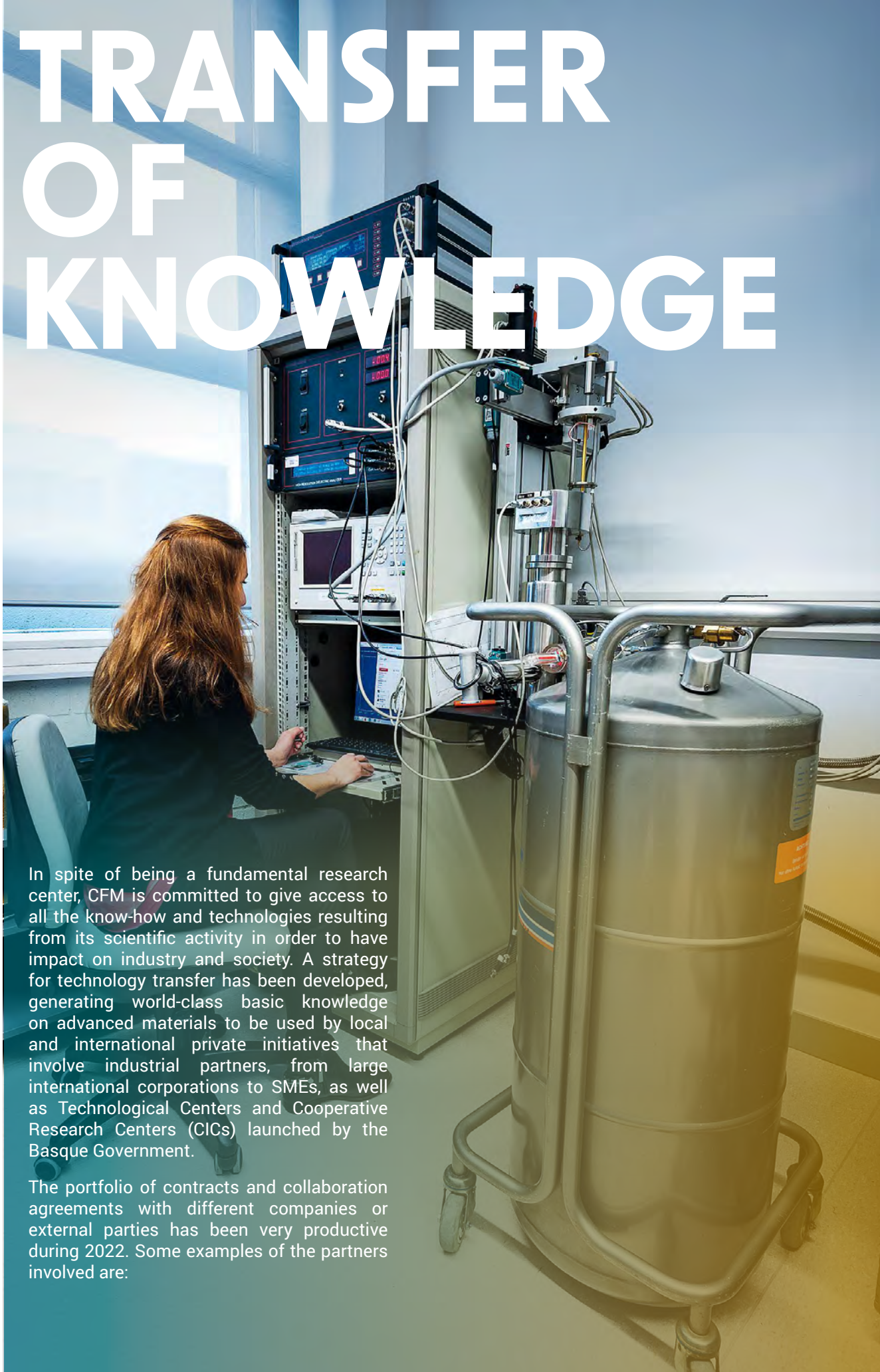
  Management Committee Member: Ángel Moreno Segurado

- **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

TRANSFER OF KNOWLEDGE



In spite of being a fundamental research center, CFM is committed to give access to all the know-how and technologies resulting from its scientific activity in order to have impact on industry and society. A strategy for technology transfer has been developed, generating world-class basic knowledge on advanced materials to be used by local and international private initiatives that involve industrial partners, from large international corporations to SMEs, as well as Technological Centers and Cooperative Research Centers (CICs) launched by the Basque Government.

The portfolio of contracts and collaboration agreements with different companies or external parties has been very productive during 2022. Some examples of the partners involved are:

Climate-KIC	Climate-KIC (EU climate innovation initiative) **Knowledge and innovation community (KIC), working to accelerate the transition o a zero-carbon, climate -resilient society.**
CADARSO	Cadarso (Gipuzkoa) **Specialists in re-carburizing additives for metallurgy**
Graphenea	Graphenea (Donostia – San Sebastián) **High quality graphene for industrial applications**
FAGOR ELECTRÓNICA	Fagor electronics (Gipuzkoa) **Desarrollo y fabricación de circuitos eléctricos híbridos semiconductor-superconductor para qubits**
janssen	Janssen Research (Belgium) **Study of dielectric properties of polymers**
basque culinary center	Basque Culinary Center Fundazioa **Food science. Physico-chemical properties of complex materials**
mugaritz	Mugaritz **Gastronomy and food science**
SIMUNE ATOMISTIC SIMULATIONS	SIMUNE ATOMICS L.T.D. **Development of software tools to improve the capabilities and the analysis of data computed with the SIESTA/TranSIESTA package**
CEMENTÁREŇ LADCE	Považská cementáreň (Slovakia) **Study of hydrated cement pastes**
Baskrete Basque Country Initiative for Cement and Concrete Research	Baskrete cross-border initiative **Concrete science and technology**
MICHELIN A BETTER WAY FORWARD	Michelin (France) **Understanding of "plasticizer effect" on concentration fluctuations and broadening of glass transition in dynamically asymmetric mixtures of interest for tire formulation**
FUNDACIÓN MUJERES POR ÁFRICA	Mujeres por África Foundation ***ELLAS INVESTIGAN* project (VI edition) to promote the leadership of African women in scientific research and technology transfer.** ***LEARN AFRICA* scholarship program for African women students**
kutxa FUNDAZIOA	Kutxa Fundazioa **Scientific cultural activities**

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

SCIENCE & SOCIETY

The goal of the science and society program at CFM is to bridge the gap between science and the public, to enhance public awareness and appreciation of science, to foster a more informed and science-literate society, and to encourage more active and meaningful participation in scientific research and innovation. By promoting dialogue and collaboration between scientists, policymakers, educators, and the general public, CFM can contribute to the development of evidence-based policies, the advancement of scientific knowledge, and the improvement of the quality of life of individuals and communities.

+ 70
activities and events,
many of them in collaboration
with other institutions

+ 10 000
participants

+ 5 600
views of the virtual contents

+ 40
researchers of CFM's staff

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**
- **Ensuring the gender balance in the talks organized**
- **Promoting the awareness on the situation**
- **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 2022 the recovery of the face to face format, combined with online visits, allowed us to reach more than **1100 students** from **28 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 little villages that usually could not travel to attend the face to face visit.

In 2022 we expanded the video collection of our premises with the virtual visit to the **Quantum nanophotonics lab.** These resources are available on our YouTube channel:

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

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

In addition to this visits, in 2021 and 2022 CFM joined the EGOKITU program. EGOKITU offers the possibility of participating in a summer science camp at the UPV/EHU devoted to motivated young students in the lasts years of their high school training. 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 28	FEBRUARY 14	MARCH 4	APRIL 1	MAY 6
Hernani BHI	La Anunciata	Jesuitak Donostia Ikastetxea	Sagrado Corazón	Santa Maria Ikastetxea
San Nikolas Ikastola	Itxaropena ikastola	Colegio Esclavas SC – Fátima	Facultad de Farmacia	
	Urretxu Zumarraga Ikastola	Nuestra señora del Carmen	Nazaret Batxilergoa	
	Larramendi Ikastola			
	Colegio Eskibel Ikastetxea			
JUNE 5	**JUNE 28**	**OCTOBER 28**	**NOVEMBER 25**	**DECEMBER 16**
EGOKITU	EGOKITU	Bideberri BHI	BHI Nazaret Batxilergoa	BHI Nazaret Batxilergoa
		Jesuitinas		Toki Ona BHI
		Erain		Colegio Vizcaya
				IES Ondarroa BHI
				Esclavas SC – Fátima
				IES Botikazar BHI
				Koldo Mitxelena
				Zubiri Manteo
				Aixerrota BHI
				Jesuitak Indautxu

ONLINE FACE TO FACE

EMAKUMEAK ZIENTZIAN 2022

emakumeakzientzian.eus

11-18/02/2022

In 2016 the United Nations General Assembly decided to proclaim 11 February as International Women's and Girls' in Science Day. To commemorate this day, the *Emakumeak Zientzian* initiative was born, to unite the forces of different research centers and science institutions of the Donostia / San Sebastian area, to make visible the activity of women in science, to break with the typically masculine roles attributed to scientific-technical activities, and to encourage the choice of scientific careers among girls and adolescents. In order to achieve these goals, #EmakumeakZientzian presented a full program that aimed at all the public, including teenager women, school kids, elder women (above 55), and also the scientific community.

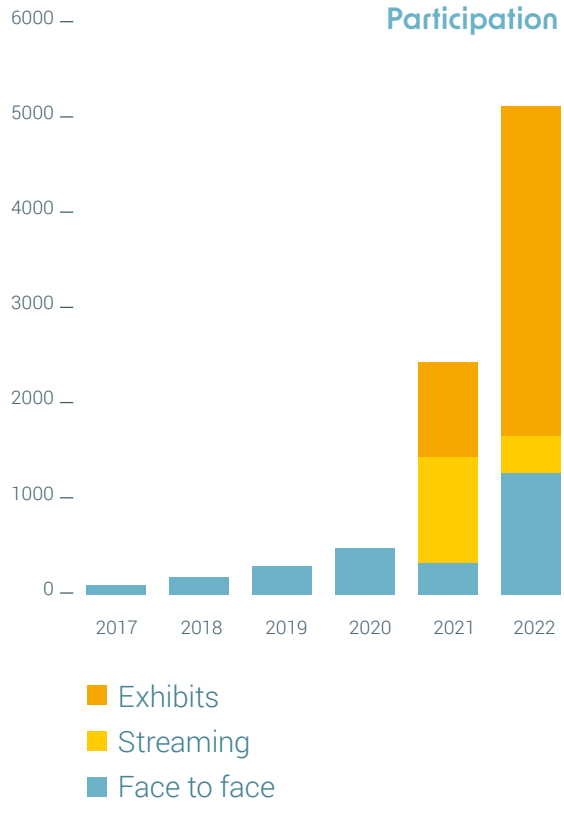
Science is indeed a girls' thing

38
Activities

+5 000
attendees

109
Volunteers

17
research centers and science-related institutions



Emakumeak Zientzian wins the 1st STEAM Euskadi Prize and the Special Mention Award for gender perspective

Emakumeak Zientzian received the first STEAM Euskadi Prize and the Special Mention Award for Gender Perspective in the category of **Most Innovative Initiative in STEAM Education promoted by organizations.** The STEAM Euskadi awards are given by the Basque Government´s Department of Education. The project was selected among 137 applications submitted to the call for proposals. More information and awards of Emakumeak Zientzian in AWARDS & MERITS section of this report.

SANCAR TEAM AT THE NANOCAR RACE II

Boule de Rangueil (Toulouse)

24-25/03/2022

The tandem from San Sebastian and Compostela SANCAR (CFM-DIPC/ CIQUS-USC) was one of the 8 teams certified to participate in the second edition of the international Nanocar Race II, the smallest car race in the world. In the Nanocar Race, the vehicles are molecules driven by the tip of a tunneling microscope over a gold surface as a circuit. The ultimate goal of this competition is to advance the development and manipulation of nanomachines capable of performing real work, such as carrying molecular weight. The winners of the Nanocar Race II were the teams that managed to cover the maximum possible distance within 24 hours: the Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA, Madrid), and the International Center for Materials Nanoarchitecture (Ibaraki, Japan).

The race was streamed and followed by more than 50.000 people all over the world.

Watch the official Nanocar Race II movie scanning this code or at **CFM's YouTube channel**

The SANCAR team

- **Design and construction of the molecule**
  Diego Peña, Jesús Castro, Dulce Rey and Manuel Vilas (CiQUS).
- **Theoretical design**
  Nicolás Lorente and Roberto Robles.
- **Experimental setup and training**
  Jan Patrick Calupitan, Martina Corso, Paula Ángulo, Tao Wang, Alejandro Berdonces, and Dimas G. de Oteiza.
- **STM microscope at CFM**
  Lucia Vitali.

PINT OF SCIENCE

pintofscience.com

Donostia / San Sebastián

09-11/05/2022

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 2022, **Carmen Gonzalez Orellana** and **Marina Peña Díaz** participated with the following talk:

The smallest trip: discovering the nanoworld

ELHUYAR ZIENTZIA AZOKA

zientzia-azoka.elhuyar.eus

Arenal (Bilbao)

02-05/06/2022

The 10th edition of Elhuyar Zientzia Azoka gathered **200 projects** developed by young students during the course. In the fair, several professional scientific stands were also present, where researchers from the CFM and POLYMAT participated under the moto "With hands on materials".

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 received the visit of the winners from Lauro Ikastola.

DONOSTIA WEEK INN 2022

donostiainn.eus/es/donostia-weekinn

22-28/10/2022

CFM regularly collaborates in the Innovation Week "Donostia WeekINN" that Fomento of San Sebastian organizes every end of October. In 2022, this collaboration was renovated again through activities for both the general public and education organized in collaboration with other institutions:

Women scientists of yesterday and today

Aquarium Donostia

26/10/2022

Featuring *Emakumeak Zientzian* 2022 edition's speakers and honored scientists.

Inside the materials world

Saint Patrick's School

20/10/2022

Nanoscience Workshop for schools organized jointly with DIPC and CIC nanoGUNE.

Can we see atoms or molecules?

Alderdi eder garden

27/10/2022

Outreach talk by CFM predoctoral researcher Paula Angulo Portugal.

"QUÉ SABEMOS DE..." TALK SERIES

cfm.ehu.es/outreach/quesabemosde

Kutxakultur plaza at Tabakalera, Donostia / San Sebastián

4, 11, 17 and 24/11/2022

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

El futuro del microbioma en la salud y la enfermedad

Daniel Ramón Vidal
Archer Daniels Midland Co.

Ser un medicamento: una carrera de obstáculos

Nuria E. Campillo and Carmen Fernández
ICMAT-CSIC and CIB-CSIC

Marte y el enigma de la vida

Juan Angel Vaquerizo
Isdefe

El oro y la neurotecnología

Ane Escobar Fernández
CFM-Gipuzkoa fellow

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

XVI SCIENCE WEEK (UPV/EHU)

Tabakalera, Donostia / San Sebastián

9-12/11/2022

From the 9th to the 12th of November 2022, CFM together with DIPC, CIC nanoGUNE and POLYMAT, joined the UPV/EHU's science week that every year gathers **thousands of visitors** to enjoy the full program of activities devoted to all public.

INSIDE THE MATERIALS STAND

In this stand predoctoral, postdoctoral and permanent researchers of CFM and the other centers collaborating in this activity, got involved in experiments and presentations to show the basis and applications of materials science and some counter-intuitive phenomena to school groups and the general public.

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.

ZIENTZIA KLUBA

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

In 2022, CFM researcher **Gabriel Molina Terriza** participated with the following talk:

Diamonds are (quantum) physics' best friends

"A LIFE IN SCIENCE" IN EUREKA! ZIENTZIA MUSEOA

Eureka! Zientzia Museoa, Donostia / San Sebastián

17 and 24/11/2022

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 2022, the following researchers from CFM joined this activity, attended by more than 300 students and 50 professionals:

- **Yuewen Fang (Oral + Poster)**
- **Claudia Borredon (Poster)**
- **Jorge Humberto Melillo (Poster)**

Available at **Eureka! Zientzia Museoa's YouTube channel** *or scanning this code*

CINEMA AND SCIENCE

Cycle organized by DIPC and Filmoteka Vasca. The following researchers from CFM joined this successful activity by participating in the presentation and discussion of the movies:

The Prize

Pedro Miguel Etxenike Landibar
13/01/2022 Artium Museoa (Vitoria - Gasteiz)
14/01/2022 Tabakalera (Donostia / San Sebastián)
15/01/2021 Fine Arts Museum (Bilbao)
18/01/2022 Golem Baionea Cinema (Pamplona)

Apollo 11

Javier Aizpurua Iriazabal
02/03/2022 Tabakalera (Donostia / San Sebastián)
27/09/2022 Teatro Filarmónica (Oviedo)

OTHER OUTREACH TALKS

Ion Errea Lope

Supereroankortasuna, markak hausten!

25/04/2022
Zientziaren Giltzak, Ondarroa

Pedro Miguel Etxenike Landibar

Small points about ethics in science

31/01/2022
Ethics in science, Nanogune Workshop 2022, Donostia

Ciencia. Economía. Salud. Cultura

03/03/2022
Beasain

CES. Ciencia, empresa y sociedad

25/04/2022
Ciclo de encuentros "Ciencia en acción". Residencia de estudiantes CSIC, Madrid

Consejos a un joven científico/a

20/05/2022
IX Jornadas Doctorales & IV Jornadas de Divulgación Científica del G9, Escuela de Ingeniería de Bilbao

100 aniversario de la biblioteca popular circulante "Menéndez Pelayo" de Castropol

11/06/2022
Castropol, Asturias

Investigación y difusión científica. Un binomio fundamental

03/06/2022
Congreso Navarro de Jóvenes Investigadores: URANIA II, Tudela

Encuentro dentro de "La semana del pensamiento"

20/09/2022
CIVICAN, Fundación Caja Navarra, Pamplona

Ciencia después del coronavirus. La sublime utilidad de la ciencia inútil

14/10/2022
Cruz Roja, Donostia

11/07-2022
Bienal física, Murcia

16/06/2022
XXVI Reunión SEUP, Pamplona

Diálogo entre Pedro Miguel Etxenike y Miguel Zugaza

11/11/2022
Global Innovation day 2022-Innobasque., Donostia

La sublime utilidad de la ciencia inútil

15/12/2022
Colloquium Marie S. Curie-CSIC, Madrid

ACTIVITY IN MASS MEDIA

Press articles
48

Online press
155

Radio
45

TV
7

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

Science, and particularly Material Physics Science, is presented in a simple and close language, in an effort to make scientific concepts and properties understandable and attractive to the general public. To this end, Idoia Mugica Mendiola, outreach manager at CFM, and Amaia Arregi Buldain, communication technician at DIPC, collaborated with "Goiz Kronika" radio show running the section "Zientzia Gosaria" (Science breakfast) that is now available as a podcast.

@CFMDONOSTIA

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

As of March 2023, CFM had more than **1400 followers in Twitter, 450 in Instagram**, and **820 in LinkedIn**. CFM's YouTube channel already contains more than 40 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.

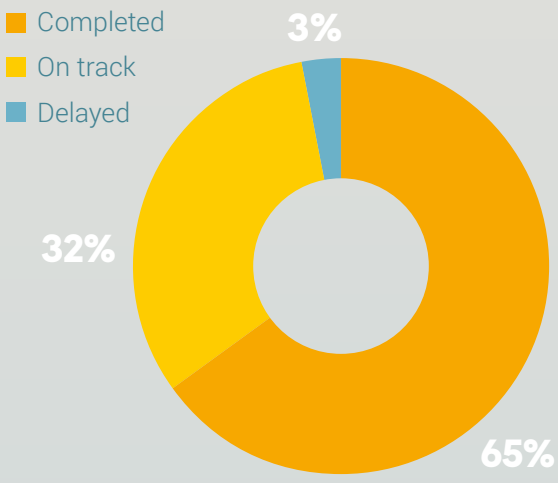
GENDER EQUALITY & DIVERSITY

SECOND YEAR OF THE IMPLEMENTATION OF THE GENDER EQUALITY PLAN

Since the need for a specific Gender Equality Plan (GEP) at CFM was first envisioned in 2017, CFM has succeeded in its development and is fully immersed in the implementation of the latter. Any worker can reach the gender equality committee at any time, in person or at genderequality.cfm@ehu.eus

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

According to the Gender Equality Plan, there were **31 actions** foreseen for this academic year, and **97% have been in place: 65 % of the actions were completed** and **32 % of them were on track.**



"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"

DIAGNOSIS 2022

CFM is committed to run an analysis of the internal situation yearly, publishing the compilation of its own indicators on gender balance. Data of 2022 is presented in the following table and figures:

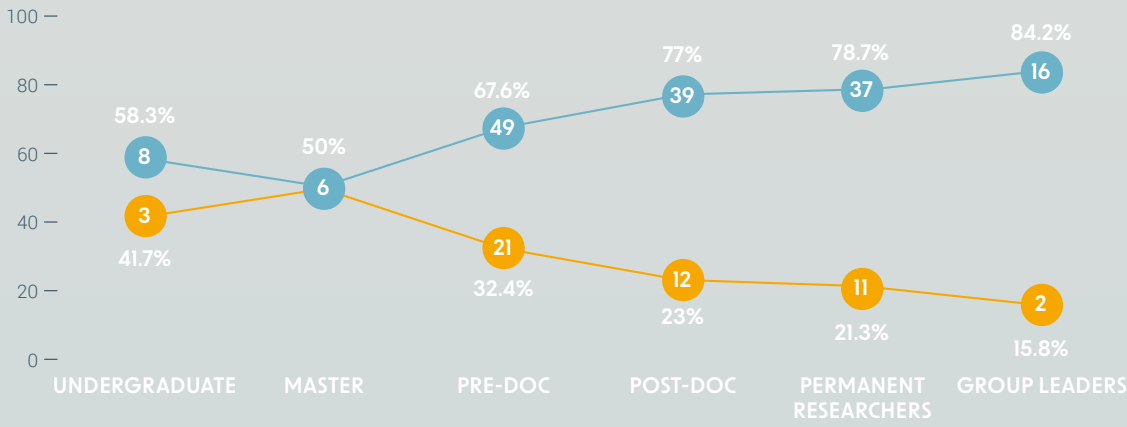
	♀	♂	
ADMINISTRATION AND SERVICES	11	10	**21**
LABORATORY TECHNICIANS	4	2	**6**
UNDERGRADUATE STUDENTS	5	7	**12**
MASTER STUDENTS	7	7	**14**
PRE-DOCTORAL RESEARCHERS	24	50	**74**
POST-DOCTORAL RESEARCHERS	14	47	**61**
PERMANENT RESEARCHERS	10	37	**48**
GUEST RESEARCHERS	18	32	**50**
OTHER GUESTS	3	0	**3**
	96	192	**288**

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

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

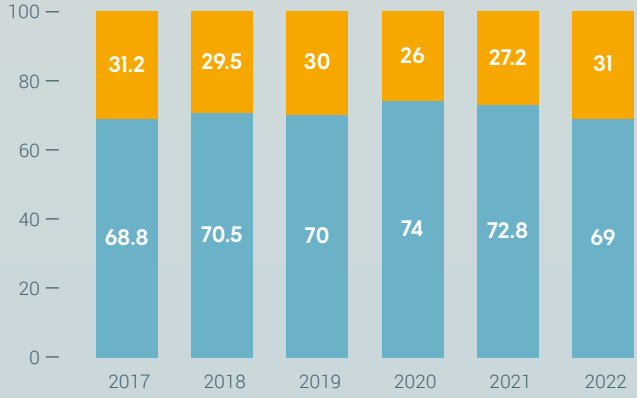
According to this data, the disproportion in the distribution of women/men in the center starts already at the earliest stage of the scientific career. Currently, 32% of the pre-doctoral researchers at CFM are women. The gender imbalance is accentuated as the responsibility for the job and level in the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



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

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



HARASSMENT PROTOCOL IN PLACE

- **Specialized training on sexual harassment** with Norma Vazquez for confidential counsellors.
- Communication campaign to socialize the protocol: The protocol was shared by email and can be found at CFM´s web page. Nevertheless, posters are present in all the building as well as in the TV screens.

AWARENESS

Since its first edition in 2017, **"Emakumeak Zientzian"** has grown to be a consolidated, award winning and participation record breaking consortia, standing out in the set of actions devoted to raise awareness on gender issues at STEM among the society. Never the less, it has also been key to build a much needed network of institutions committed to work together in breaking the gender divide in the scientific and technological field. **Emakumeak zientzian** has been further described in depth in sections 13- Science and Society and 15- *Awards and merits* of this report and constitutes the main achievement regarding social awareness on gender issues.

Never the less, the aim of the plan also includes carrying out activities to raise **awareness** on gender issues specifically among CFM's staff. In this regard, among other actions, in 2022 the Gender Equality committee decided to launch the **"CFM's good practice guideline"** devoted to CFM´s community, that is available at CFM´s web page.

CREATING A DIVERSE WORKFORCE

- **Work-life balance survey** to all CFM community, to identify specific needs.
- Reviewing **recruitment and promotion processes** in a specific report.
- **Unconscious biases effects in recruitment and promotion processes:** Training devoted to all decision making bodies, i.e. group leaders, project PIs, and permanent researchers.

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

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

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

In the framework of this initiative, the program Ellas Investigan (Women investigate) promoted by the foundation Women for Africa, brings an African researcher to carry out a six-month research stay at CFM. This type of extended research visit was also supported by The Provincial Council of Gipuzkoa in 2022 through a 20 000€ collaboration grant. The selected researcher was **Florette Fobasso Mbognou** from University of Dschang-Cameroon (Physics department), who will join the group of **Ion Errea** (Quantum Theory of Materials) in May 2023.

PRIDE IN SCIENCE
Looking Inside to get Outside

Since 2019 and under the slogan **"Pride in Science"** *(Harrotasuna Zientzian / Orgullo en Ciencia),* CIC nanoGUNE, DIPC and CFM jointly praise the International Day of Pride in STEM which is celebrated the 18th November internationally. The initiative aims to give visibility to the LGBTQIA+ collective in science, actively contribute to breaking old stereotypes and celebrate diversity as a pillar in the future of science.

To celebrate Pride in Science Day 2022, the event **"Looking inside to get outside"** devoted to the scientific and technological community was organized.

All the members of the collective as well as allies working in the STEM field in Donostia / San Sebastián were invited to participate in an informal work coffee guided by members of the Pride in Science alliance. In this safe and private space, ideas, opinions, and experiences were exchanged and later collected in a summary of what was discussed. One of the main conclusions was the need to build a community and to that end a WhatsApp group was created as a fast and easy way to join the so far created network.

29 people from
14 research institutions participated.

MENTAL HEALTH

At CFM we are actively working to create a healthy work environment for everyone at all levels. We are sincerely concerned about the well-being of our staff, especially those at the earlier stages of their careers.

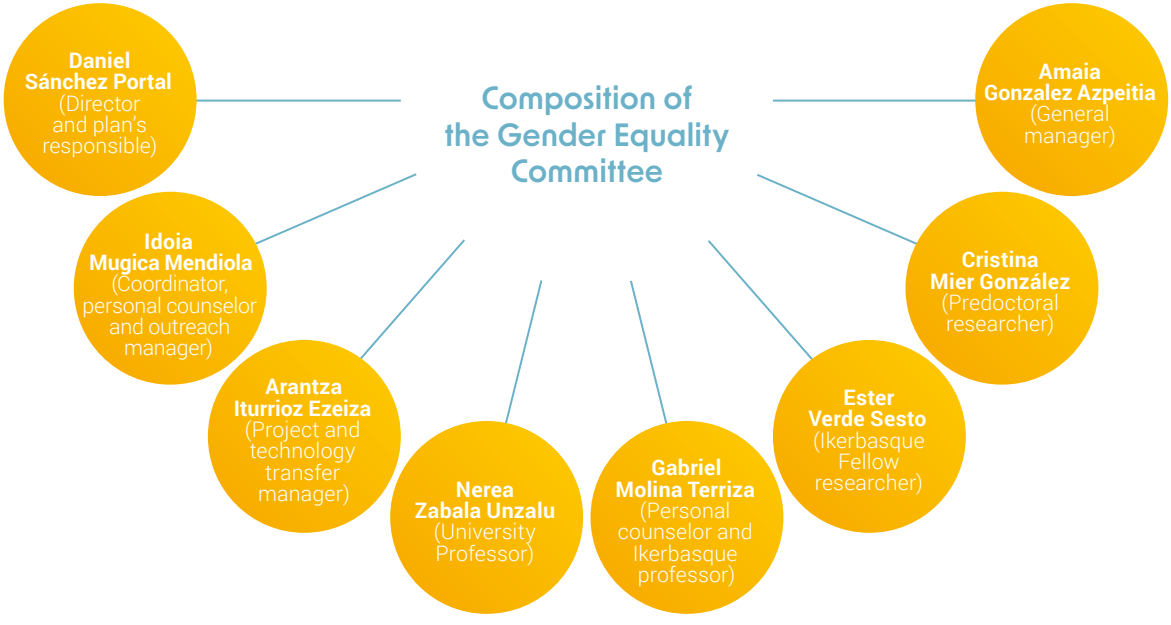
To be able to make a diagnosis of the situation and level of satisfaction of **PhD candidates** at CFM regarding mental health and work/life balance, in 2022 we launched an **anonymous survey**, the results (report and analysis) of which were shared through our community and can be consulted at CFM´s web page.

Furthermore, an **Emotional intelligence workshop**, devoted to researchers at the early stages of their careers was organized (see the "Transferable Skills program" in section 10 of this report for further information).

CONSOLIDATED AND REGULAR ACTIONS

- Ensuring the representation of 50% of women in all the dissemination lectures organized by CFM.
- Encouraging women researchers to participate in the different dissemination programs, especially those aimed at children, families and young people.
- Using the CFM social media to highlight the research results of the women scientists working at CFM.
- Promoting other initiatives that share the fundamental contributions of women in science, such as "Women with Science" by Marta Macho (Chair in Scientific Culture), "Women and Girls in Science Day", Donostia WeekInn, etc.

The implementation of the GEP is driven by the Gender Equality Committee, formed by staff members representing CFM's different working areas. The Committee remains active in the critical phase of the implementation that will last 4 years. During 2021 Elhuyar, which is approved by Emakunde (the Basque Institute for Women) to give technical Gender Equality support to institutions, has been giving technical advice and supporting CFM in this major task, and continues to do so in 2022.



AWARDS & MERITS

2.3 MILLION EUROS ERC STARTING GRANT TO SARA BARJA MARTÍNEZ, WITH HER COSAS PROJECT

The European Research Council has awarded the prestigious ERC Starting Grant to the Ramon y Cajal UPV/EHU researcher at the CFM, Sara Barja Martínez, with her **COSAS** Project

The **2.3 million** euros grant will enable the COSAS project, whose mission is to develop new, more efficient and economical catalysts to produce green hydrogen by exploring electrolysis from seawater – thus avoiding the costly process of purifying seawater to optimize hydrogen production – to be developed over the next five years.

The ERC Starting Grant, is one of the most competitive and prestigious grants awarded by the European Research Council, with more than more than 4000 proposals received, and only 397 selected. This program highlights the promising work of the brightest young scientists so that they have the freedom to develop their own innovative line of research and contribute to expanding the frontiers of knowledge.

The 2.3 million euros awarded to Dr. Barja will enable the COSAS (Controlling Oxygen Selectivity at Atomic Scale) project to be developed over the next five years, which seeks to study hydrogen production processes in depth from a fundamental point of view, in order to contribute to their sustainability. The exploration of alternative energy sources and fuels to fossil fuels is in line with the Sustainable Development Goals (SDGs) set by the United Nations, and with the Basque Hydrogen Strategy defined by the Basque Government's energy agency. This project, led by the UPV/EHU and the CFM, will give a major boost in this regard.

9 MILLION EUROS FOR THE ALBA SYNCHROTRON NEW BEAM LINE

3Sbar (Surface Structure and Spectroscopy at 1 bar) is the name of the next ALBA beamline that will be extremely useful to provide answers to environment protection. 3Sbar is a unique instrument that will provide unprecedented insight on the understanding of fundamental processes in catalytic reactions. The project, funded by the Recovery, Transformation and Resilience Plan within the framework of the NextGenerationEU, will enter operation in 2026.

The scientific case of the project and its conceptual design has been elaborated by Professor **Enrique Ortega** (CFM, UPV/EHU), Dr. Xavier Torrelles (Institut de Ciència dels Materials de Barcelona, CSIC) and Dr. Eduardo Solano (ALBA Synchrotron), with the support and collaboration of many ALBA colleagues from the Experiments, Accelerator, Computing and Engineering Divisions.

This new beamline will be key to understand the correlation between chemical reactions and structural changes at atmospheric pressures, which represents a big step ahead for fundamental research in surface chemistry and catalysis. It will allow to get a deep insight in the basic processes determining the efficiencies of catalysts under industrial operating pressures.

3Sbar will also be extremely useful to provide answers to environmental protection, challenges such as CO_2 reduction, the wastewater treatment, the development of environmentally friendly industrial catalytic processes or the recycling of greenhouse gases.

Its estimated cost is 9 million euros, which have been granted by the Ministry of Science and Innovation through the European Recovery and Resilience Facility within the NextGenerationEU Program. It covers the construction and staff positions needed for designing and operating this new beamline. Two new job positions are open now. The detailed design of the beamline starts now, the construction is expected to finish in 2025 and the instrument will be in operation by 2026.

EMAKUMEAK ZIENTZIAN TWICE AWARDED IN 2022:

Winner of the STEAM Euskadi Prize and the Special Mention Award For Gender Perspective given by the Basque Government's Education Department

Winner of the special recognition by fomento san sebastián at the 9th edition of innovation week

Emakumeak Zientzian [Women in Science] received the first **STEAM Euskadi Prize** and the **Special Mention Award for Gender Perspective** in the category of Most Innovative Initiative in STEAM Education promoted by other organizations. The STEAM Euskadi awards are given by the Basque Government´s Department of Education. The project was selected among 137 applications submitted to the call for proposals.

Fomento San Sebastian also gave a special recognition to this initiative in at the 9th edition of the innovation week. The Councillor for Economic Development, Marisol Garmendia, presented this year's award to Emakumeak Zientzian, for making the activity of women in science visible.

The award and the recognition acknowledge the progress made by the Emakumeak Zientzian initiative since the first edition in 2017, and the work of all the people and organizations involved in its development. Emakumeak Zientzian has been proposing an extensive program of activities geared towards society as a whole to mark 11 February, International Day of Women and Girls in Science, with emphasis on particularly important groups in order to promote equal access and professional development in STEM disciplines.

"If there is one thing we are clear about, it is that breaking the gender divide in the scientific and technological field requires a global awareness; a global approach," stressed Mónica Moreno, head of projects and communication at POLYMAT and coordinator of the 2022 edition of Emakumeak Zientzian.

"This initiative has also made it possible to build a network of scientists committed to internal change in scientific and technical organizations in order to break the gender divide and achieve full and equal professional development for everyone," added Idoia Mugika, Outreach manager at CFM and coordinator of the 2023 edition of Emakumeak Zientzian

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