



Materialen Fisika Zentroa  
Centro de Física de Materiales  
Materials Physics Center

# ACTIVITY REPORT

# 2020



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# ACTIVITY REPORT 2020

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**CFM**  
**Centro de Física de Materiales**  
Materialen Fisika Zentroa  
Materials Physics Center





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# FOREWORD

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



Iñaki Juaristi Oliden, Vicedirector

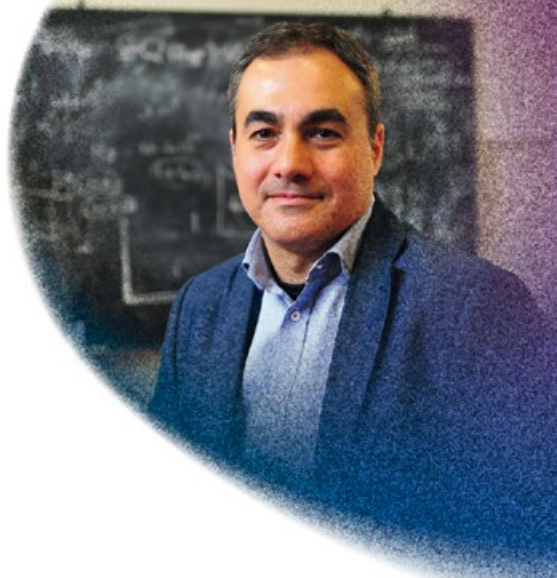
2020 has been a complicated and strange year. For several months, many of us looked around us with a feeling of disbelief, helplessness and sadness as we saw our certainties, routines and, ultimately our way of life tragically transformed due to the Covid-19 pandemic. We have witnessed how many of our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

However, from the point of view of science and research activity, the year 2020 has been somewhat more ambiguous. Of course, the pandemic had a negative initial impact. The *Centro de Física de Materiales* (CFM), following the regulation imposed by the University of the Basque Country (UPV/EHU), remained closed and without face-to-face activity for almost two months. During the second half of May, we resumed our activity using a system that combined teleworking with face-to-face activity in shifts, which allowed us to maintain a low occupancy of our facilities. Other measures were imposed, such as the mandatory use of the mask, the closure of communal areas such as the cafeteria and the auditorium, and courses, workshops and scheduled meetings were suspended, etc. Thanks to these measures, and to the discipline and stoicism with which all the staff adopted these measures, it was possible to prevent the appear-

ance of large outbreaks of Covid-19 in the CFM. There have only been isolated cases that were quickly reported, the people involved swiftly confined in their homes, and the possible transmission in the center was avoided. Fortunately, none of these cases had serious consequences. For this civic, responsible and understanding attitude, I want to warmly congratulate all the CFM staff. Finally, in October 2020 the work shifts were definitively abandoned, since they considerably hindered the activity in the laboratories. However, to this day, part of the staff still carries out part of their activities by teleworking.

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

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



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

### Daniel Sánchez Portal, Director

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

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

Autumn 2020 started with the replacement of Andrés Arnau Pino as Deputy Director of CFM by Iñaki Juaristi Olliden. We really want to thank Andrés for all his great work during the last five years and particularly for his support during the last year, when he had to act both as CFM Deputy Director and Acting Administration Manager. Ano-

ther important event in Autumn 2020 was the official retirement of our colleague and friend Pedro Echenique Landiribar, a teacher both in science and in life for many of us. He is one the main personalities behind CFM and had a key role in the creation and development of CFM and its research environment (DIPC, nanoGUNE, etc.). He continues with his research, science popularization and science policy advising activities as an Emeritus Professor at UPV/EHU.

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

The brilliant trajectory and international visibility gained by CFM in the last years was only possible thanks to the commitment of all CFM personnel and to the decisive and continuous support of the three key institutions behind CFM: CSIC, UPV/EHU and the Basque Government. We also count on the support from Gipuzkoa Province Government. With these allies we are fully confident that we will keep producing basic science at the highest level.

Thank you all for your commitment and support.

Daniel Sánchez Portal  
Iñaki Juaristi Olliden

# GOVERNANCE

## CFM

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

### CURRENT DIRECTION BOARD OF CFM

**Director:** Daniel Sánchez Portal

**Vice director:** Iñaki Juaristi Oliden

**Secretary:** Amaia González Azpeitia

### SCIENTIFIC BOARD OF CFM

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



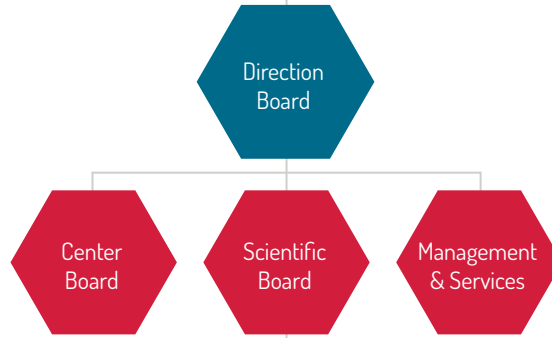
# CFM

CSIC

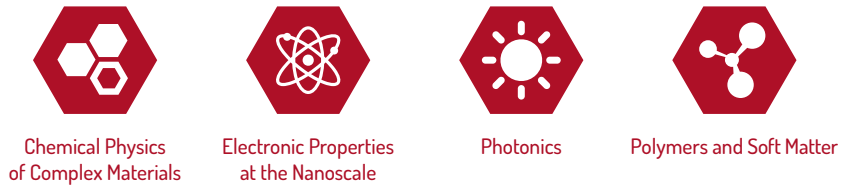
UPV/EHU



## Board of Governance



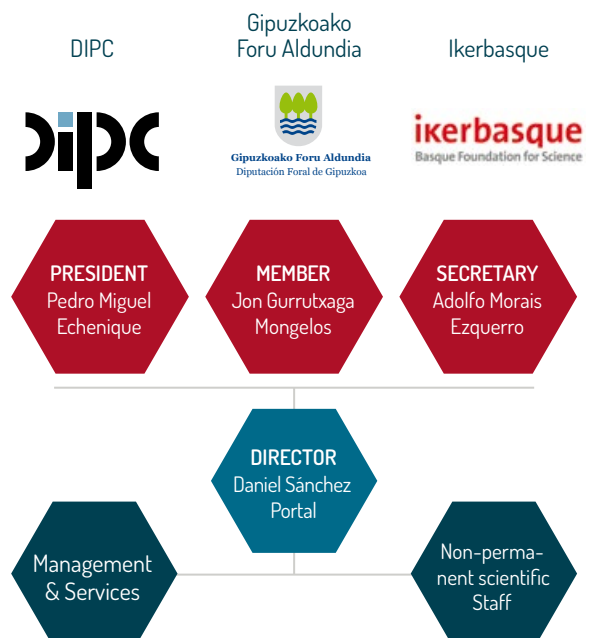
## Research Lines



## MPC-BERC

The association Materials Physics Center (MPC) is a non-profit organization declared as Basic Excellence Research Center (BERC) which is intrinsically united to CFM, and shares its goals and scientific activity, serving as an instrumental body in a totally synergistic and combined activity. The body of governance of the MPC-BERC is constituted by the Basque Foundation for Science (Ikerbasque), the Gipuzkoa Provincial Council (*Gipuzkoako Foru Aldundia*), and the Donostia International Physics Center (DIPC), who appoints the scientific director of the association. The combined and united strategic activity of both CFM-MPC is ensured by the joint appointment of the same person as director of both institutional bodies.

## MPC - BERC



# PROFILE

## SCIENTIFIC COMMUNITY

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Researchers in  
Action

194

18

Research Groups



## TRAINING

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12

PhD Theses  
defended

17

Master Theses  
Defended<sup>1</sup>

3

Undergraduate  
Projects

## RESEARCH OUTPUT

---

ISI Publications

217

Citations<sup>2</sup>

13 021

International Collaborations

81%

Q1 Publications<sup>3</sup>

69%

H Index

133

D1 Publications

43%



**49%**  
of the Research Community  
is international

Researchers from  
**36**  
countries

## ACTIVITIES AND EVENTS

Seminars

**14**

Conferences, Workshops  
and Courses<sup>4</sup>

**3**

Science and Society

**28** Activities  
**10 000** Attendees

## PROJECTS AND FUNDING

Ongoing Projects

**82**

Funding

**5 088 818,50 €**

<sup>1</sup> In the framework of the nanoscience master or supervised by CFM staff

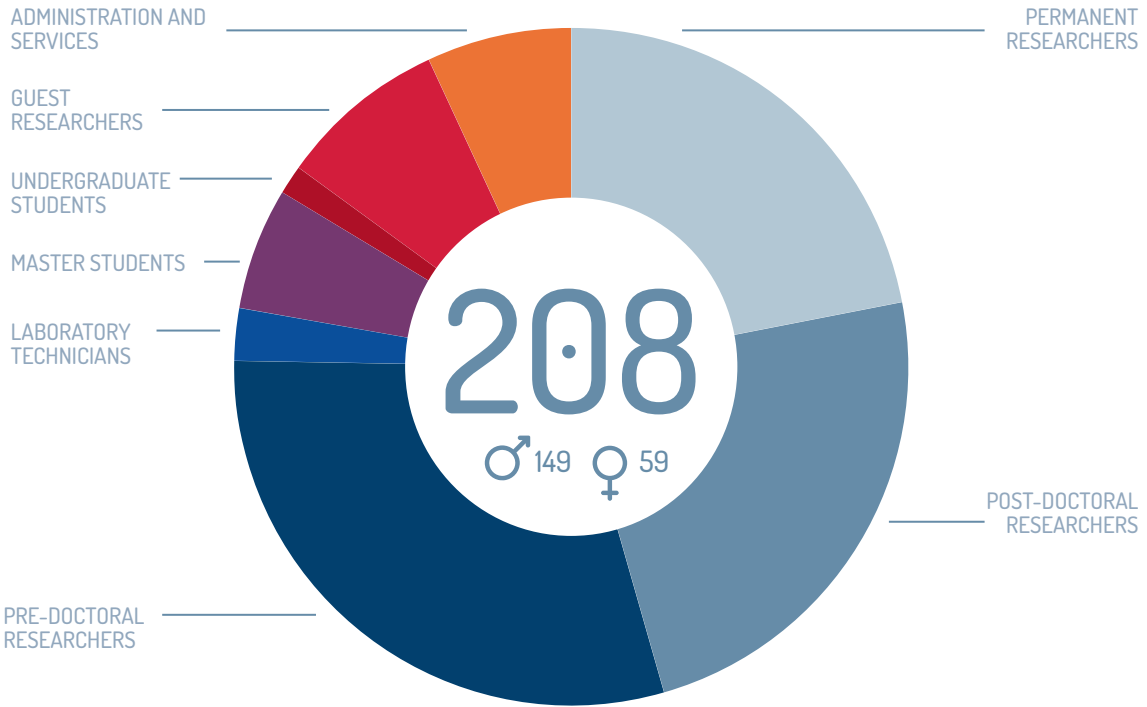
<sup>2</sup> Including Physical Review B: 81%

<sup>3</sup> Source: Web of Science Core Collection as of April 2021

<sup>4</sup> Due to the pandemic, 6 events scheduled in 2020 had to be cancelled.

# PEOPLE

## ALL THE CFM COMMUNITY



CFM Staff

# 181

Researchers in Action

# 194<sup>3</sup>

Permanent Researchers	46
Post-doctoral Researchers	49
Pre-doctoral Researchers	62
Laboratory Technicians	5
Master students <sup>1</sup>	12
Undergraduate students <sup>2</sup>	3
Guest Researchers	17
Administration and Services	14
<b>Total</b>	<b>208</b>

<sup>1</sup> Four of those receive scholarships during their stay at CFM and are considered staff

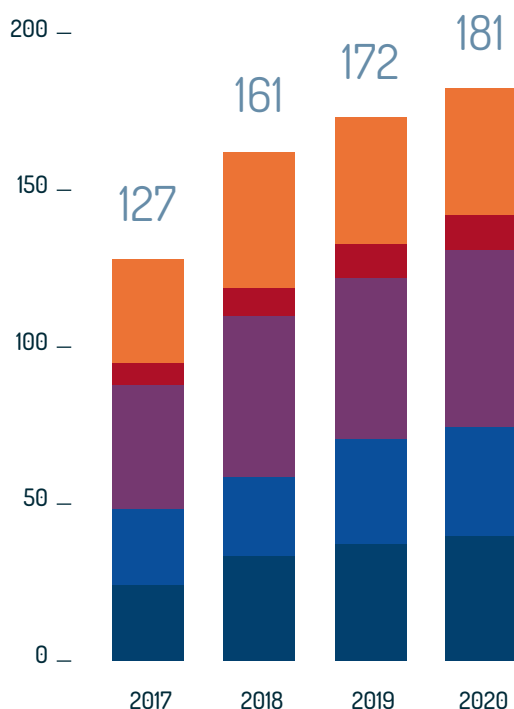
<sup>2</sup> One of those receive scholarships during their stay at CFM and is considered staff

<sup>3</sup> Including Guest researchers, undergraduate and master students

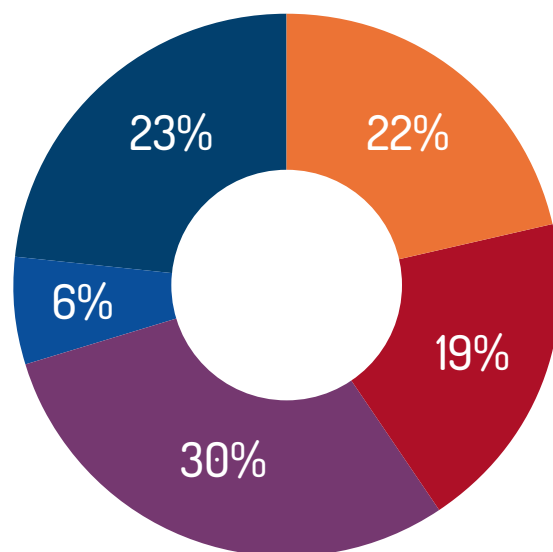
## DISTRIBUTION OF CFM STAFF according to the origin of their financial support

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

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



Distribution of CFM staff in percentage according to the origin of their financial support in 2020



## DIRECTION BOARD

**Director:** Daniel Sánchez Portal

**General Manager:** Amaia González Azpeitia

**Before September 2020**

**Vicedirector:** Andrés Arnau Pino

**From September 2020**

**Vicedirector:** Iñaki Juaristi Oliden



## ADMINISTRATION AND SERVICES

### Administration

Adolfo del Arco García, Administrative, CSIC

Amaia Gonzalez Azpeitia, Administration Manager, CSIC

Ane Iturriza Semperena, Administrative, MPC

Arantza Iturrioz Ezeiza, Project and Technology Transfer Manager, MPC

Elixabet Sarasketa Zabala, Project and Technology Transfer Manager, MPC

Idoia Mugica Mendiola, Outreach Manager, MPC

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

Laura Martín Montañez, Outreach Internship, MPC

María Formoso Ferreiro, Administrative, MPC

Marta López Pérez, Administrative, MPC

Txema Ramos Fernandez, Administrative, CSIC

### Computing and IT Services

Iñigo Aldazabal Mensa, Computer Center Manager, CSIC

Ioritz Paulis Garmendia, IT Systems Technician, MPC

### Maintenance

Juan Manuel Burgos Jiménez, MPC

## LABORATORY TECHNICIANS

Amaia Iturrospe Ibarra, CSIC

Luis Botana Salgueiros, CSIC

María Isabel Asenjo Sanz, MPC

María Lourdes Leza Fernández, UPV/EHU

Silvia Arrese-Igor Irigoyen, CSIC



# RESEARCHERS

Research Line:



## Chemical Physics of Complex Materials

### 01 Gas/Solid Interfaces

#### Permanent Researchers

Iñaki Juaristi Oriden, Associate Professor, UPV/EHU  
Maite Alducin Ochoa, Tenured Scientist, CSIC  
Ricardo Díez Muiño, Research Scientist, CSIC

#### Post-doctoral Researchers

Alberto Pablo Sánchez Muzas  
Raúl Bombin Escudero

#### Pre-doctoral Researchers

Alberto Rodríguez Fernández  
Alfredo Serrano Jiménez  
Auguste Tetenoire

#### Guest Researchers

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

### 02 Quantum Phenomena on Surfaces

#### Permanent Researcher

Nicolás Lorente Palacios, Research Scientist, CSIC

#### Ikerbasque Fellow

Deungjang Choi, MPC

#### Post-doctoral Researchers

Felix Mouhat  
Roberto Robles Rodríguez  
Vladimir Zobac

#### Pre-doctoral Researchers

Cristina Mier González  
José Reina Gálvez

### 03 Nanophysics Lab

#### Permanent Researchers

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

#### Ramon y Cajal Researcher

Sara Barja Martínez

#### Post-doctoral Researchers

Andrew P. Weber  
Djuro Bikaljevic  
Jan Patrick Calupitan  
Khadiza Ali  
Laura Fernández Gómez-Recuero

Marco Gobbi (Ikerbasque fellow on leave at CIC nanoGUNE)

Maxim Ilin  
Rishav Harsh  
Tao Wang  
Vahagn Mkhitarian

#### Pre-doctoral Researchers

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

#### Guest Researchers

Lorena Glatthaar, Master Student  
Naoya Sumi, Pre-doctoral Researcher

## 04 Modelisation and Simulation

### Permanent Researchers

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

### Post-doctoral Researchers

Carlos García Fernández  
Mikhail Otrokov

### Pre-doctoral Researchers

Joseba Goikoetxea Perez  
Masoud Mansouri

### Guest Researchers

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

## 05 Spectroscopy at Atomic Scale

### Permanent Researcher

Lucia Vitali, Ikerbasque Professor, UPV/EHU

### Post-doctoral Researchers

Ana Barragán Durán  
Jie Hou

### Pre-doctoral Researcher

Francisco Javier Manterola Maraño

## 06 Theoretical and Computational Chemistry

### Permanent Researcher

Pedro Braña Coto, Research Scientist, CSIC

Research Line:



## Electronic Properties at the Nanoscale

## 07 Electronic Excitations in Surfaces and Nanostructures

### Permanent Researchers

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

### Post-doctoral Researchers

Ilya Nechaev  
Marta Z. Pelc

### Pre-doctoral Researchers

Mikel Arruabarrena Larrarte  
Raúl Guerrero Avilés

### Guest Researcher

Jozef Janovec, Pre-doctoral Researcher



## 08 Quantum Theory of Materials

### Permanent Researchers

Aitor Bergara Jauregui, Associate Professor, UPV/EHU

Ion Errea Lope, Associate Professor, UPV/EHU

Jose María Pitarke de la Torre, University Professor, UPV/EHU

### Post-doctoral Researcher

Raffaello Bianco

### Pre-doctoral Researchers

Antonella Meninno

Francesco Belli

Iñigo Robredo Magro

Josu Diego López

Martín Gutiérrez Amigo

Oscar Rodríguez Ballesteros

Pugeng Hou

Unai Aseguinolaza Aguirreche

### Guest Researcher

Lorenzo Monacelli, Pre-doctoral Researcher

## 09 Mesoscopic Physics

### Permanent Researchers

F. Sebastián Bergeret Sbarbaro, Tenured Scientist, CSIC

Vitaly Golovach, Ikerbasque Associate, UPV/EHU

### Post-doctoral Researcher

Stefan Ilic

### Pre-doctoral Researchers

Alberto Hijano Mendizabal

Cristina Sanz Fernández

Mikel Rouco Martin

Xian-Peng Zhang

## 10 Nano-Bio Spectroscopy

### Permanent Researcher

Ángel Rubio Secades, University Professor, UPV/EHU

## 11 Souza Research Group

### Permanent Researcher

Ivo Souza, Ikerbasque Professor, UPV/EHU

### Post-doctoral Researcher

Julen Ibañez Azpiroz

### Pre-doctoral Researcher

Miguel Ángel Jiménez Herrera

### Guest Researcher

Cheol-Hwan Park, Senior Scientist

## 12 Ceramic and Cement-Based Materials

### Permanent Researcher

Jorge Sánchez-Dolado, Tenured Scientist, CSIC

### Post-doctoral Researcher

Guido Goracci

### Pre-doctoral Researcher

Mohammad Rahjoo

### Guest Researchers

Mohammadreza Izadifar, Pre-doctoral Researcher

Valentina Musumeci, Pre-doctoral Researcher

Research Line:



# Photonics

## 13 Theory of Nanophotonics

### Permanent Researchers

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

### Post-doctoral Researchers

Eduarne Gorraitz Eusa  
Mario Zapata Herrera  
Luca Bergamini  
Roberto Álvarez Boto

### Pre-doctoral Researchers

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

### Guest Researchers

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

## 14 Nanomaterials and Spectroscopy

### Permanent Researchers

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

### Post-doctoral Researchers

María Sanromán Iglesias  
Thomas Hendel

### Pre-doctoral Researchers

Alba María Jumbo Nogales  
Joscha Kruse  
Sara Luisa Marina Barbier

### Guest Researcher

Aimar Marauri Iriberrí, Undergraduate Student

## 15 Laser Physics and Photonic Materials

### Permanent Researcher

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

## 16 Quantum Nanophotonics Laboratory

### Permanent Researcher

Gabriel Molina Terriza, Ikerbasque Professor, MPC

### Post-doctoral Researchers

Francesc Monrabal Capilla  
Juan José Miguel Varga  
Rubén González Moreno

### Pre-doctoral Researchers

Iker Gómez Viloría  
Jon Lasa Alonso  
Martin Molezuelas Ferreras

### Master Student

Harriet Kumi

Research Line:



# Polymers and Soft Matter

## 17 Polymers and Soft Matter

### Permanent Researchers

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

### Ikerbasque Fellows

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

### Post-doctoral Researchers

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

### Pre-doctoral Researchers

Agustín Blazquez Martín  
Amaia Matanza Corro  
Ane Izaskun Aranburu Leiva  
Claudia Borredon

Davide Arena  
Javier Martínez Sabando  
Jokin Pinacho Olaciregui  
Jordan Ochs  
Jorge Humberto Melillo  
Julen de la Cuesta Leone  
Maiara Aime Iriarte Alonso  
Mariarita Paciolla  
Matteo Sanviti  
Maud Formanek  
Mohammed El Amine Hanifa  
Numera Shafqat

### Master Student

Jean Pierre Inchaustegui Revoredo

### Undergraduate Student

Julen Olasagasti Imizcoz

### Guest Researchers

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

## 18 Quantum Beams and Sustainable Materials

### Permanent Researcher

Felix Fernández Alonso, Ikerbasque Professor, MPC

### Post-doctoral Researcher

Kacper Druzbecki

### Pre-doctoral Researcher

Balthasar Braunewell

### Guest Researcher

Mohammed Ali Al Assiri, Master Student

# OTHER POSITIONS

## Associate Professor

Isabel Tellería Echeverría, UPV/EHU

## Senior Scientists

Dimas García de Oteyza Feldermann, Ikerbasque Professor, DIPC

Fabienne Barroso Bujans, Ikerbasque Professor, DIPC

Miguel Moreno Ugeda, Ikerbasque Associate, DIPC

## Post-doctoral Researchers

Wen Wan, DIPC (Miguel Moreno's group)

James Lawrence, DIPC (Dimas García de Oteyza's group)

## Pre-doctoral Researchers

Alejandro Berdonces Layunta, DIPC (Dimas García de Oteyza's group)

Mohammed Sabri Gamal Mohammed, DIPC (Dimas García de Oteyza's group)

Pablo Herrero Gómez, DIPC (Dimas García de Oteyza's group)

Paul Lukas Dreher, DIPC (Miguel Moreno's group)

## Master Students

Andrés Felipe Bejarano Sanchez, MPC / DIPC

Nathaniel Andrés Capote Robayna, MPC / DIPC

## Guest Researcher

Jan Holec, Post-doctoral Researcher (Dimas García de Oteyza's group)

# EXTERNAL ADVISORY COMMITTEE



Professor  
**Peter Saalfrank**

*Institut für Chemie,  
Universität Potsdam, Germany*  
Expertise in the line of Chemical  
Physics of Complex Materials

## Honors and Awards

Chair of Theoretical Chemistry, *Universität Potsdam* (2008-2010); Elected 'Fachkollegiat' (Referee Board Member) of *Deutsche Forschungsgemeinschaft* (German Research Council, DFG), "*Fachkollegium Festkörper- und Oberflächenchemie: Theorie und Modellierung*" (Solid State and Surface Chemistry: Theory and Modelling) (2004-2008, 2016-2019).

## Research Interests

Theoretical Surface Science; System-bath quantum dynamics; Laser-driven electron dynamics; Theoretical photophysics and chemistry; Electronic structure theory.



Professor  
**Francisco  
J. García Vidal**

Department of Theoretical  
Condensed Matter, *Universidad  
Autónoma de Madrid, Spain*  
Expertise in the line of Photonics

## Honors and Awards

Director of the IFIMAC- Condensed Matter Physics Center (*María de Maeztu Center*); Prof. García Vidal is one of the most prestigious researchers in Photonics in the world. He knows well the reality of research in Spain, and the local boundaries for science and technology, particularly the evaluation systems in both CSIC and the Ministry of Science, Innovation and Universities.

## Research Interests

Photonics and nanophotonics.



Emeritus Professor  
**Antonio  
Hernando Grande**

*Universidad Complutense de  
Madrid, Spain*  
Expertise in the line of Electronic  
Properties at the Nanoscale

## Honors and Awards

Director of *Instituto de Magnetismo Aplicado (IMA)* from 1989 to 2017; *Académico Numerario de la Real Academia de Ciencias Exactas, Físicas y Naturales*; Honoris Causa Doctor by the UPV/EHU and by the Cantabria university; Gold Medal by the *Real Sociedad Española de Física*; Miguel Catalán research award by the Autonomous Community of Madrid; Fellow of the American Physical Society; Dupont science award; *Juan de la Cierva* national research award.

## Research Interests

Magnetism and related areas. He combines basic research of magnetic materials with projects in applied research.



Professor  
**Dieter Richter**

Jülich Center for Neutron  
Science (JNSC) and  
Institute of Complex  
Systems, Jülich, Germany  
Expertise in the line of  
Polymers and Soft Matter

## Honors and Awards

Director of the Institute for Neutron Scattering at the FZJ (1989-2014); Chair at the Materials Physics Department of the University of the Basque Country founded by the Bank of Bilbao Vizcaya (1997); "*Staudinger-Durrer Prize of the ETH*" (2015); "*Walter Hälgl Prize*" of the European Neutron Scattering Association (2009); "*Erwin-Schrödinger Award*" (2002); "*Max-Planck Award*" (1990) among others.

## Research Interests

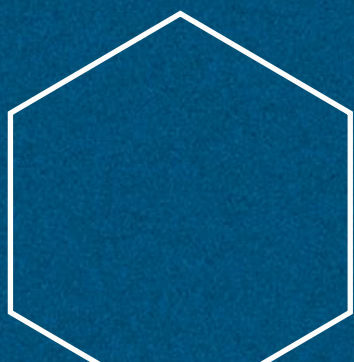
Structure and Dynamics of Polymers and Soft Matter; Neutron Techniques and Instrumentation.



# RESEARCH LINES & GROUPS

CFM focuses on the study of four main strategic aspects of matter that cover some of the main structures and systems in advanced materials research, within the general objective to target excellence in the research on materials physics, namely: Molecules, Solid State Systems, Photons, and Soft Matter. The research activities in the center have thus been structured during the last years into the corresponding four research lines that give response to the aforementioned targets. The current research lines in the center are: (i) **Chemical Physics of Complex Materials**, (ii) **Electronic Properties at the Nanoscale**, (iii) **Photonics** and (iv) **Polymers and Soft Matter**.

Gathered under these four research lines, at CFM the fundamental unit of organization is the research group, although the structure remains fully horizontal, actively seeking cross-linked multidisciplinary research.



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

Sixteen of these groups develop their activity in the premises of CFM in Donostia / San Sebastián, while the laboratories of the “Laser Physics and Photonics Materials” group are located at the Engineering School of Bilbao (UPV/EHU), and the “Nano-Bio Spectroscopy” group is located in the *Joxe Mari Kortza* (UPV/EHU) research building, in the *Ibaeta* Campus in Donostia / San Sebastián.

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



# CHEMICAL PHYSICS OF COMPLEX MATERIALS

The research line *Chemical Physics of Complex Materials* addresses the structural and electronic properties of complex nanostructured materials, particularly in the presence of molecules.

Six research groups are included in this research line, with a high degree of complementarity. Four of the groups devote their activity to the ab-initio theoretical study of electronic structure and dynamical processes of nanostructures and molecules, as well as to condensed matter states, which show interesting topological properties. These groups are the "Gas/Solid Interfaces" group (01), the "Quantum Phenomena on Surfaces" group (02), the "Modelisation and Simulation" group (04), and the "Theoretical and Computational Chemistry" group (06).

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

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



## 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 cal-

culations to describe the interaction dynamics in such complex systems. Particular attention is paid to the development of theoretical models able to describe the non-adiabatic contributions and the energy dissipation channels that come into play, because they can drastically change the output of the dynamics.

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



2

## Quantum Phenomena on Surfaces

Group Leader: Nicolás Lorente Palacios, Research Scientist, CSIC

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

from semiconductors and metals to superconductors.

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

3

## Nanophysics Lab

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

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

to mention the exploration of such surface properties and phenomena using curved crystals of varied nature as substrates, defining a radically new experimental approach that is becoming the hallmark of the group.

The NPL holds some of the most modern and complete set of surface-sensitive techniques and instrumentation, combined in a variety of multi-technique ultra-high-vacuum setups, distributed in five different laboratory rooms.

4

## Modelisation and Simulation

Group Leader: Daniel Sánchez Portal, Research Professor, CSIC

The activity of the "Modelisation and Simulation" group focuses on the theoretical study of the electronic and structural properties of complex materials, clean and decorated surfaces, and nanostructures. It pursues the following objectives: (i) to develop the basic theory and ab-initio simulation tools in order to study the behavior of different nanoelectronic devices, particularly those based on graphene derivatives, (ii) to study the optical properties of complex organic/inorganic interfaces, (iii) to study the

magnetic properties of different nanostructures, ranging from one dimensional systems to coordination networks and multilayer heterostructures at surfaces, and (iv) to continue to foster the development of the SIESTA code.

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

5

## Spectroscopy at Atomic Scale

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

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

functional groups, and (iv) two dimensional properties emerging in layered materials.

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

6

## Theoretical and Computational Chemistry

Group Leader: Pedro Braña Coto, Research Scientist, CSIC

The group's research is focused on the theoretical investigation of excited state reactivity and dynamics in complex molecular systems. Researchers at this group use theory and simulation to characterize fundamental aspects of

the photophysics and photochemistry of these systems with emphasis on charge and energy transfer and transport processes in novel materials with applications to nanoelectronics, organic photovoltaics, and lighting.



# ELECTRONIC PROPERTIES AT THE NANOSCALE

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

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



## 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) nanos-

tructures of carbon nanotubes, inorganic nanotubes and minerals with silicate chains.

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

8

## Quantum Theory of Materials

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

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

compounds with interesting properties fully ab initio.

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

9

## Mesoscopic Physics

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

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

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

ical tools and computational codes to investigate the electronic response of solids and nanostructures to external electromagnetic fields has been settled in this group. The main research interests of this activity are as follows: (i) foundations of time-dependent density

functional theory for biophysics, (ii) foundations of the many-body theory, (iii) electronic and thermal transport, (iv) theory of open quantum systems, and (v) strong light-matter interactions and optimal control theory.

In recent years, the main research activities on these topics include new developments within the many-body theory and TDDFT, covering ab-initio descriptions of electron excitations, optical spectroscopy, time-resolved spectroscopies, and lifetimes. Novel techniques

to calculate total energies have been also developed, assessing exchange correlation (XC) functionals for TDDFT calculations. Improvements on transport theory within the real-time TDDFT formalism have also been achieved. Moreover, the electronic and optical properties of solids, nanostructures (in particular nanotubes, nanowires and semiconducting -clusters-) and biomolecules is also tackled in the group. All these activities have resulted in the establishment of the European Theoretical Spectroscopy Facility (ETSF).

11

## Souza Research Group

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

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

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

12

## Ceramic and Cement-Based Materials

Group Leader: Jorge Sánchez Dolado, Tenured Scientist, CSIC

The group researches a variety of properties of cement-based and ceramic materials experimentally and theoretically. Combining knowledge from different disciplines like solid-state physics, soft-matter physics, geochemistry and chemical engineering, the "Ceramic and Cement-based Materials" group focuses on the computational design and synthesis of new ceramic and cement-based materials with lower CO<sub>2</sub> footprint.

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

ture and properties of cement-based materials, (ii) the implementation of new technologies in hydrothermal and supercritical fluids (SCF) for the ultra-fast synthesis of ceramic nanoparticles, (iii) the development of new sintering methodologies through the use of autoclaves or microwaves that allow notable energy savings and a drastic reduction of CO<sub>2</sub> emissions, and (iv) the development of energy storage solutions derived from cement-based materials, including both chemical storage (batteries) and thermal storage systems (TES) applications.



# PHOTONICS

The research line on *Photonics* deals with the experimental and theoretical study of the interaction of radiation with matter from different and complementary approaches: (i) the interaction of light with metallic and semiconductor nanostructures to confine and engineer electromagnetic fields in the nanoscale, (ii) the optical properties of new materials and elements that provide improved properties in a variety of lasing effects, as well as the design of novel photonic structures that provide laser confinement for bioimaging, and (iii) spectroscopy and photonic applications of nanoscale functional units, including different types of low-dimensional systems. Several research activities along these lines are developed by the groups listed below, including theoretical and experimental activities.

13

## Theory of Nanophotonics

**Group Leader: Javier Aizpurua Iriazabal, Research Professor, CSIC**

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

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

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

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## Nanomaterials and Spectroscopy

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

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

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

15

## Laser Physics and Photonic Materials

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

The activity of the “Laser Physics and Photonic Materials” group concentrates most of the research efforts on the study of optoelectronic properties of new materials and structures for solid state lasing and photonic crystal properties.

In recent years, the following specific objectives have been pursued on this topic: (i) the investigation on rare earth-doped vitroceraamics for integrated optics applications, (ii) the study of the laser emission processes in dye-doped micro-nano structured hybrid materials

for optoelectronic and biomedical applications, (iii) the synthesis and development of new eutectic materials for biomedical applications, (iv) the study of slow light in micro-nano structured materials with forbidden band gaps, (v) the experimental and theoretical study of light generation in rare-earth doped micro-nano-crystalline dielectric powders for infrared random lasers, (vi) the study of laser-induced refrigeration in rare earth-doped micro-nano structured materials, and (vii) the design and making up of an optical wave guide writing system by using a femtosecond laser.

# Quantum Nanophotonics Laboratory

Group Leader: Gabriel Molina Terriza, Ikerbasque Professor, MPC

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

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

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



## POLYMERS AND SOFT MATTER

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



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## Polymers and Soft Matter

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

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

different length and time scales is demanded.

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

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## Quantum Beams and Sustainable Materials

Group Leader: Félix Fernández Alonso, Ikerbasque Professor, MPC

The “Quantum Beams and Sustainable Materials” group makes extensive use of beams of quantum particles like neutrons or photons in tandem with computational materials modelling to interrogate, understand, and design novel functional materials for energy applications and sustainability. This research program is underpinned by the development of new techniques and methodologies

for materials discovery, in close collaboration with leading neutron and X-ray laboratories from around the globe.

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

# HIGHLIGHTS

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1

# Quantum corrections in the dynamics of hydrogen molecules at surfaces

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

Physical Chemistry Chemical Physics 22, 22805 (2020)

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

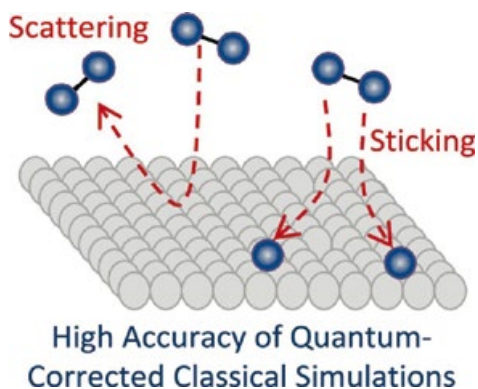
Elementary processes arising in gas/solid interfaces are ever-present in our daily life as well as in many industrial applications. The oxidation and corrosion of surfaces, the catalytic converters used in cars, the surface doping of semiconductors, or the industrial production of most synthetic compounds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

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

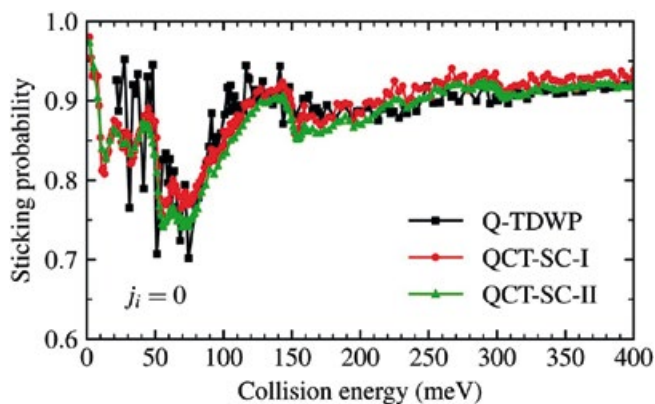
In this work, the authors improve over a classical trajectory method by including quantum corrections. The interaction between the molecules and the surface are described by density functional theory. They assign statistical weights to classical paths on the basis of two semiclassical corrections: Gaussian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

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

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



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



## 2

# Vibron-assisted spin excitation in a magnetically anisotropic molecule

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

Nature Communications 11, 1619 (2020)

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

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

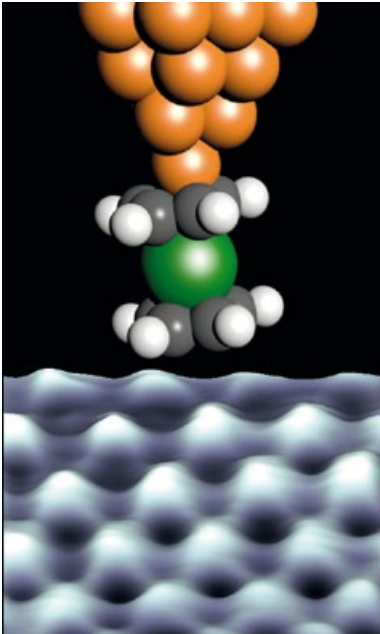
In the present work Bachelier et al. show that the molecule can also have vibrational excitations, and when the electrons have enough energy to simultaneously excite vibrational and spin degrees of freedom, they do it with an enormous efficiency. This is really

surprising because inelastic electron transmission is usually thought to be less efficient than the corresponding elastic process, let alone to have two simultaneous excitations of the spin-excitation signal.

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

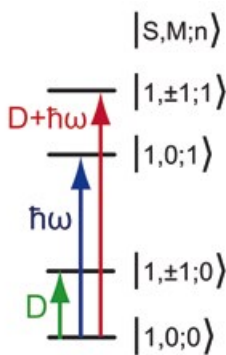
“Electronic correlations  
give rise to very complex  
molecular excitations”

(a)

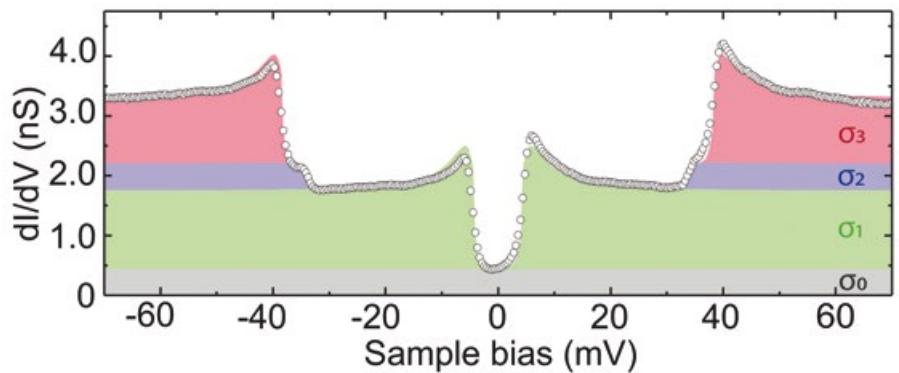


**Figure:** (a) A nickelocene molecule (C<sub>10</sub>H<sub>10</sub>) trapped by an atom of the STM tip over a surface. (b) Energy levels with spin and vibrational degrees of freedom.  $D$  is the magnetic anisotropy equal to 3.8 meV and the frequency ( $\hbar\omega$ ) is equal to 34 meV. (c) Differential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

(b)



(c)



## 3

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

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

Angewandte Chemie-International Edition 59, 20037 (2020)

CO oxidation ( $2\text{CO} + \text{O}_2 \rightarrow \text{CO}_2$ ) on platinum metal surfaces is a model heterogeneous gas/surface catalytic reaction. Here, researchers investigated CO oxidation at different Pt crystal planes around the (111) direction, using a curved Pt surface. They surprisingly found that the ignition occurs simultaneously at all surface facets.

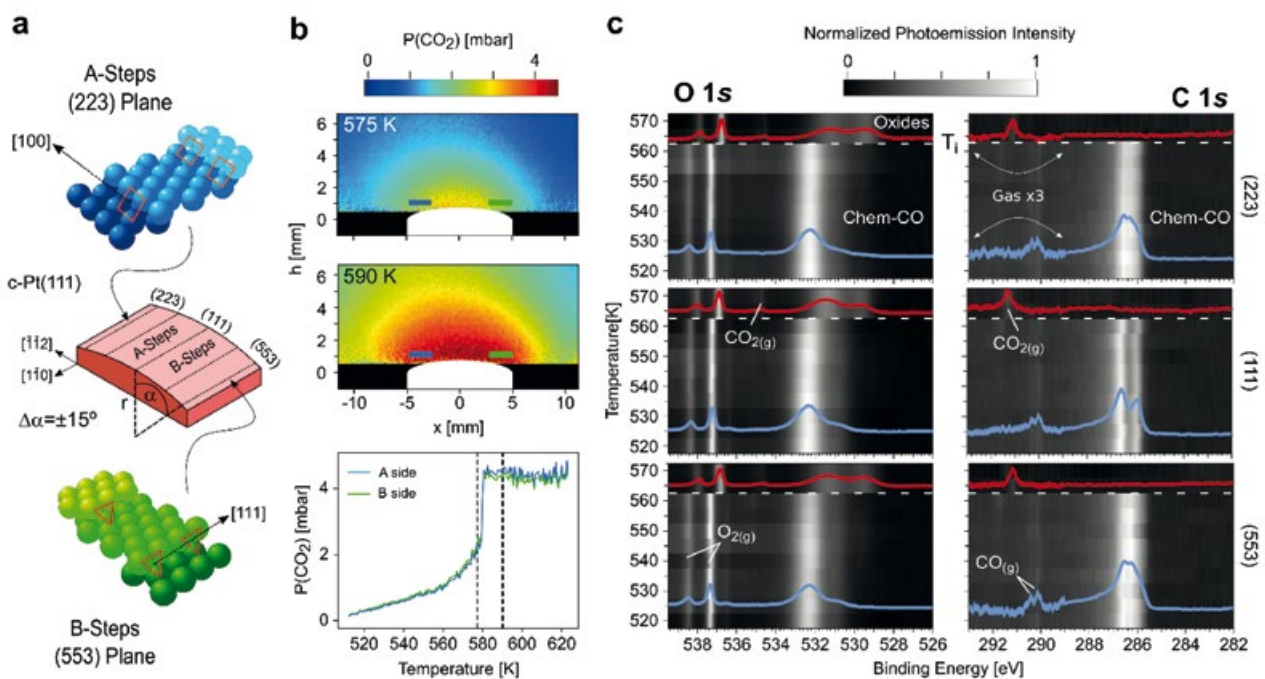
Platinum (Pt) is of utmost importance as a catalyst for car exhaust cleaning or for the water gas shift reaction, whereas Pt crystal surfaces are model systems for investigating the catalytic CO oxidation at the atomic scale. During decades, researchers have studied the sequential and simultaneous interaction of CO and O<sub>2</sub> with Pt under high vacuum conditions, providing a detailed description of fundamental steps in the reaction: O<sub>2</sub> dissociation, CO and O chemisorption, and CO-O interaction. Lately, a deeper insight is being gained through techniques operating at millibar pressures, such as Near Ambient Pressure X-ray Photoemission Spectroscopy (NAP-XPS).

All these studies agree on the fundamental picture: the abrupt transition at "ignition", from the low-temperature poisoning stage, when CO covers the surface and blocks the reaction, to the high-temperature active stage, when CO is displaced from the surface by chemisorbed oxygen. However, the mechanism of such CO → O transition, and the differences among crystal planes, of enormous relevance in nanoparticle catalysis, remain unknown.

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



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



**Figure:** Simultaneous ignition of the CO oxidation on a curved Pt surface. (a) Sketch of the c-Pt(111) curved crystal sample featuring A-type and B-type vicinal surfaces. (b) Top-middle, two-dimensional snapshots of Planar Laser Induced Fluorescence (PLIF) of  $\text{CO}_2$  for a 6 mbar  $\text{CO}:\text{O}_2$  mixture in front of the c-Pt(111) surface, right before (575 K) and after (590 K) light-off, illustrating the simultaneous ignition of the CO oxidation at all points. Bottom,  $\text{CO}_2$  PLIF signal measured at the stepped A- and B-edges of the sample, marking the ignition at  $\sim 580$  K. (c) O 1s (left) and C 1s (right) photoemission intensity images measured at three different points on the c-Pt(111) sample exposed to  $\sim 1$  mbar  $\text{CO}:\text{O}_2$  during a heating cycle. Vanishing of CO and emergence of oxygen-related species mark an abrupt, simultaneous ignition of the reaction.

# 4

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

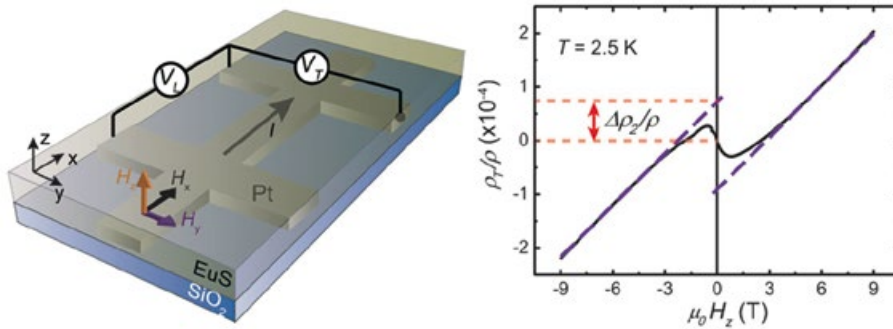
**Gomez-Perez JM, Zhang XP, Calavalle F, Ilyn M, Gonzalez-Orellana C, Gobbi M, Rogero C, Chuvilin A, Golovach VN, Hueso LE, Bergeret FS, and Casanova F.**

Nano Letters 20, 6815 (2020)

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

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

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



**Figure:** Scheme of the fabricated Hall-bar devices and transverse resistivity measurement in Hall configuration. Dash purple lines correspond to the linear fit performed at large magnetic fields and extrapolated to zero. The red arrow shows the clear  $\Delta\rho_2/\rho$ .

group at CIC nanoGUNE. Generation of spin current in these devices was studied via measuring of Spin Hall magnetoresistance (SMR) at low temperatures and in high magnetic fields. The theoretical model developed by researchers of the Mesoscopic Physics group at CFM allowed to quantify all three parameters defining the spin current through the interface: the spin-sink conductance  $G_s$ , which originates when the electron spins of the nonmagnetic metal are collinear with the MI magnetization and both the real and imaginary parts of the spin-mixing conductance  $G_{\uparrow\downarrow} = G_r + i^*G_i$ , which originate from torques that the electron spins of the nonmagnetic metal exert to the magnetization of the MI when they are noncollinear.  $G_r$  is determined by the Slonczewski (or damping-like) torque, a quantity crucial for the spin-torque devices. On the other hand,  $G_i$  quantifies the exchange field between the electrons of the nonmagnetic

metal and the magnetic moments of the MI, exerting a field-like torque when spin accumulation is induced. This interfacial exchange field is very relevant in different areas. For instance, when the nonmagnetic metal is a superconductor, it leads to a spin-splitting field, even in the absence of an external magnetic field.

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

## 5

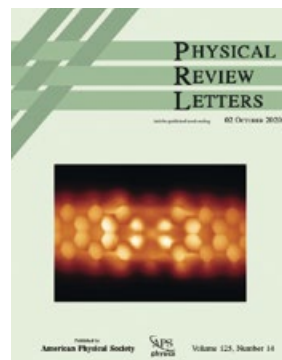
# Magnetism of topological boundary states induced by boron substitution in graphene nanoribbons

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

Physical Review Letters 125, 146801 (2020)

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

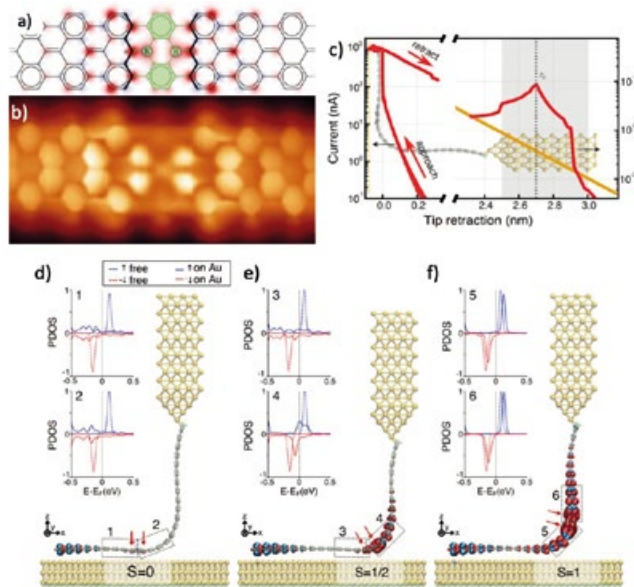
GNRs can be classified according to the topology of their electronic band structures. This allows predicting the appearance of zero-energy states bound at the boundaries between GNRs of different topological classes or at the edges of topologically non-trivial ribbons. These localized states give rise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



The authors of this work show that magnetic boundary states can be created in the interior of a GNR simply by embedding substitutional heteroatoms in the carbon backbone. A pair of boron atoms substituting carbon turns out to act as a physical termination for the topological valence band of the ribbon (7-AGNR) and, hence, creates end states that are singly occupied and spin polarized. First indications of the presence of magnetism were given by the appearance of characteristic Kondo peaks in electrical transport experiments performed at CIC nanoGUNE. Transport was measured through boron-substituted GNRs suspended between the tip and the sample of a Scanning Tunneling Microscope (STM). These observations were rationalized in terms of the theory and first-principles simulations performed at CFM and DIPC,

which predicted for each isolated boron pair a  $S=1$  spin state as well as a strong dependence on the spacing between pairs. The interaction between two of such topological defects was further explored, outlining a route to engineer topological spin chains, with the promising tunability of their magnetism by modifying their spacing.

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



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

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

## 6

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

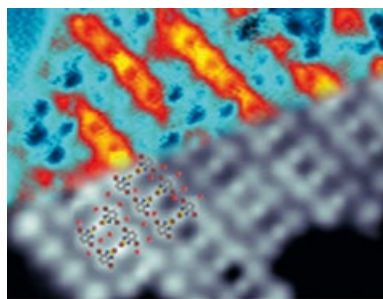
**Barragan A, Sarasola A, and Vitali L.**

Angewandte Chemie-International Edition 59, 15599 (2020)

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

In the last decade, a considerable scientific attention has been devoted to the formation of ordered organic structures ensuring molecular functionalities and good electrical properties. In this context, a valuable approach was offered by Ullmann cross-coupling reactions where halogenated molecules catalyzed by metal surfaces promoted the synthesis of extended structures through the molecular polymerization. This chemical approach results in good mechanical and electrical contacts between components. In this collaborative work between the Donostia International Physics Center (DIPC), the University of the Basque Country (UPV/EHU) and CFM, the authors show that the electron conductance of benzothiadiazole molecules, extensively used in electronics, can be enhanced even before their polymerization. Indeed, despite the formation of a porous network, two adjacent, periodic and isoenergetic contributions, namely a molecular electronic resonance and the con-

finied surface-state, sum-up forming one-dimensional conductance channels, observable in energy-resolved maps of a 2D-metal-organic network. Though they do not contribute directly to the conductance, the adsorption configurations of Br atoms, inorganic byproduct of the redox-reacted 4,7-dibromobenzo[c]-1,2,5-thiadiazole molecules on the copper surface critically control the channel continuity. These halogen atoms enable the delocalization of the molecular electronic resonance into a continuous channel acting on the confinement of the Cu(110) surface state on the pores. Small displacements of the Br atoms change the local surface potential misaligning the energy levels and creating discontinuity into the channels. This work opens new perspectives on charge-transport mechanisms controlled by an order-disorder transition determined by the movement of single atoms limiting carrier's mobility in two-dimensional organic networks.



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

# 7

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

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

Nature Communications 11, 4821 (2020)

Using Angle Resolved Photoemission Spectroscopy (ARPES) and *ab initio* calculations, Hirahara et al. have studied the molecular beam epitaxy grown heterostructure  $\text{Mn}_4\text{Bi}_2\text{Te}_7/\text{Bi}_2\text{Te}_3$  achieved by self-organization of the Mn and Te adatoms co-deposited on  $\text{Bi}_2\text{Te}_3$ . The authors reveal a sizable Dirac point gap and study its temperature evolution.

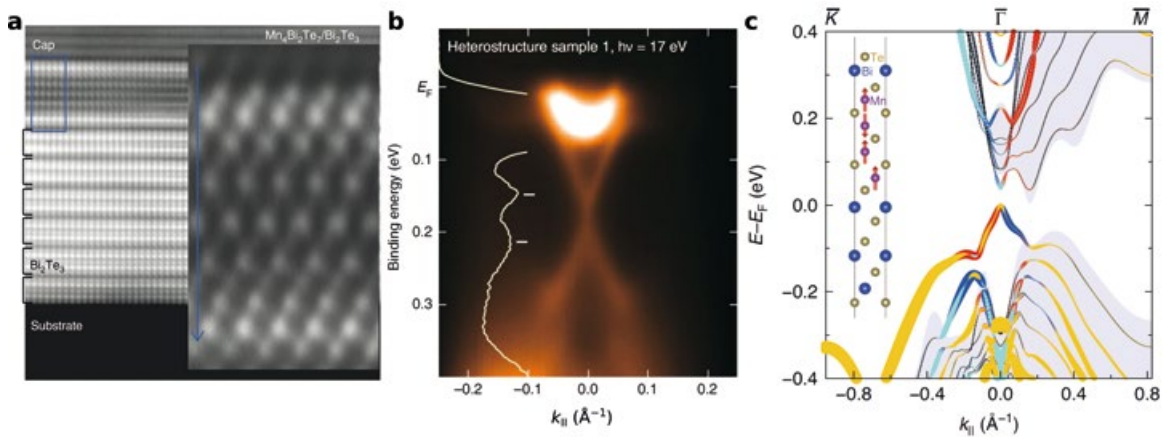
Although the interfaces between trivial magnetic and topological nonmagnetic insulators have recently attracted a great deal of attention, no photoemission evidence of the Dirac point gap opening in the topological interface state has been reported. To bridge this gap, the authors have synthesized a novel magnetic topological heterostructure with a built-in interface achieved via self-organization of the MnTe film inside of the  $\text{Bi}_2\text{Te}_3$  surface quintuple layer block (e.g., Te-Bi-Se-[MnTe]-

Bi-Te), where the magnetic film has adopted its bulk-like (NiAs-like) structure, see Figure (a). The resulting structure can be written as  $\text{Mn}_4\text{Bi}_2\text{Te}_7/\text{Bi}_2\text{Te}_3$ . Strikingly, the realization of this scenario leads to a unique situation when the heterostructure's magnetic part is based on a material that intrinsically does not show Van der Waals bonding (MnTe), but turns out to be Van der Waals coupled to a topological insulator substrate.

ARPES measurements of  $\text{Mn}_4\text{Bi}_2\text{Te}_7/\text{Bi}_2\text{Te}_3$  reveal a massive Dirac cone with a gap of 40-75 meV at 16 K (Figure b). The system showed long-range magnetic order with a critical temperature of about 20 K. *Ab initio* calculations predict a complicated magnetic configuration for  $\text{Mn}_4\text{Bi}_2\text{Te}_7/\text{Bi}_2\text{Te}_3$  combining both ferromagnetic and antiferromagnetic couplings between adjacent layers (Figure c, inset). Surface electronic structure calculations confirm the existence of the gapped Dirac cone for these crystal and magnetic structures (Figure c). Further, by tracing the temperature evolution, they find the Dirac point gap to gradually decrease with increasing temperature, with a transition from a massive to a massless Dirac cone occurring around 200–250 K. Thus, these results show for the first time that the Dirac

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

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



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



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# 8

## Quantum fluctuations sustain the record superconductor

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

Nature 578, 66 (2020)

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

The 250 kelvin ( $-23^\circ\text{C}$ ) obtained in  $\text{LaH}_{10}$ , the usual temperature at which home freezers work, is the hottest temperature for which superconductivity has ever been observed. The possibility of high-temperature superconductivity in  $\text{LaH}_{10}$ , a superhydride formed by lanthanum and hydrogen, was anticipated by crystal structure predictions back in 2017. These calculations suggested that above 230 gigapascals a highly symmetric  $\text{LaH}_{10}$  compound (Fm-3m space group), with a hydrogen cage enclosing the lanthanum atoms (see figure), would be formed. It was calculated that this structure would distort at lower pressures, breaking the highly symmetric pattern. However, experiments performed in 2019 were able to synthesize the highly symmetric compound at much lower pressures, from 130 to 220 gigapascals,

and to measure superconductivity around 250 kelvin in this pressure range. Therefore, the crystal structure of the record superconductor, and thus its superconductivity, remained not entirely clear.

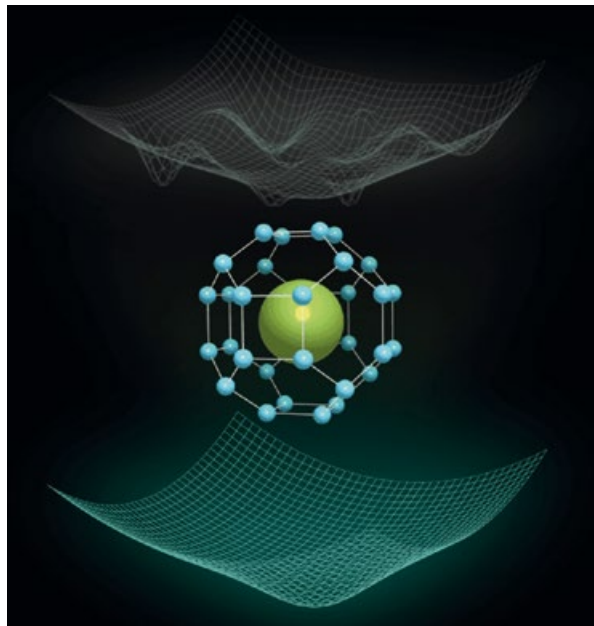
Now, this work shows that atomic quantum fluctuations “glue” the symmetric structure of  $\text{LaH}_{10}$  in all the pressure range in which superconductivity has been observed.

In more detail, the calculations show that if atoms are treated as classical particles, that is, as simple points in space, many distortions of the structure tend to lower the energy of the system. This means that the classical energy landscape is very complex, with many minima (see figure), like a highly deformed mattress because many people are standing on it. However, when atoms are treated like quantum objects, which are described with a delocalized wave function, the energy landscape is completely reshaped: only one minimum is evident (see figure), which corresponds to the highly symmetric Fm-3m structure.

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

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

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



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

# 9

## A Josephson phase battery

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

Nature Nanotechnology 15, 656 (2020)

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

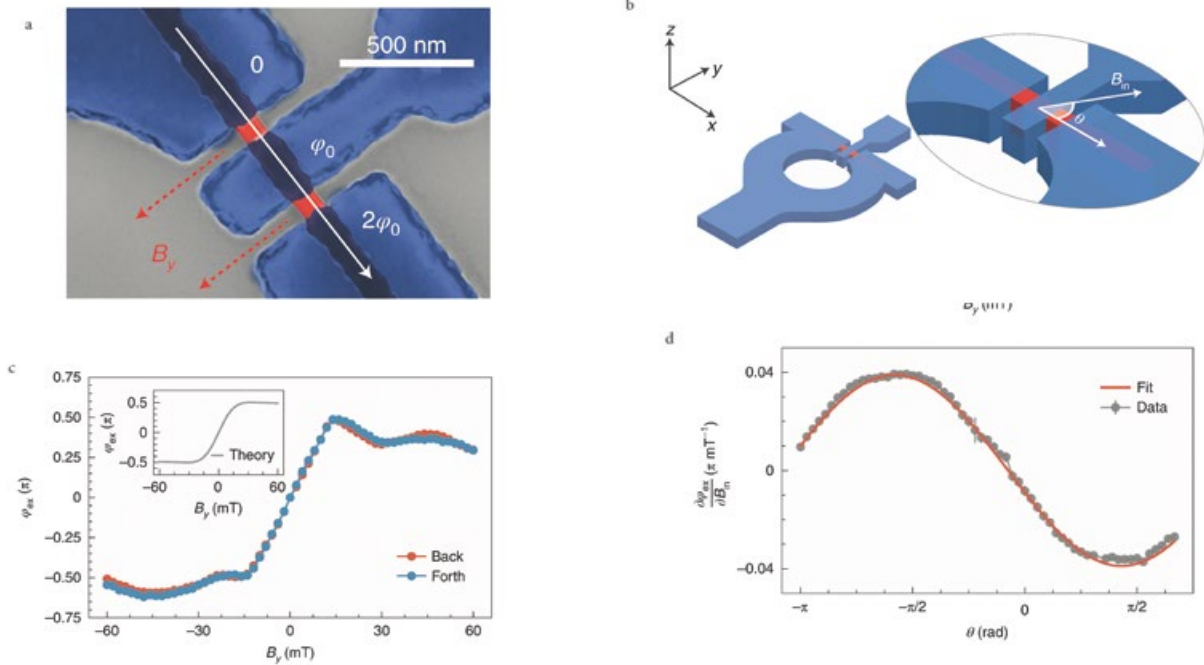
A classical battery converts chemical energy into a persistent voltage bias that can power electronic circuits. We denote a phase battery as a quantum device that provides a persistent phase bias to a quantum circuit's wave function. It represents a key element for quantum technologies based on phase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

The device is shown in figure (a). It consists of an n-doped InAs nanowire (red) with unpaired-spin surface states, proximitized by Al superconducting leads (blue). The authors found that the ferromagnetic polarization of the unpaired-spin states is efficiently converted into a persistent phase bias  $\varphi_0$  across the wire, leading to the anomalous Josephson effect. The phase bias can be controlled by an external magnetic field [figure (b)], achieving a continuous tuning of  $\varphi_0$  [figure (c)]. Hence, it is possible to charge and discharge the quantum phase battery. The observed symmetries of the anomalous Josephson effect in the vectorial magnetic field agree with the theoretical predictions calculated by the authors [figure (d)] in a previous work<sup>1,2</sup>.

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

<sup>1</sup> Bergeret FS, and Tokatly IV  
Theory of diffusive  $\varphi_0$  Josephson junctions in the presence of spin-orbit coupling.  
EPL 110, 57005 (2015).

<sup>2</sup> Konschelle F, Tokatly IV, and Bergeret FS  
Theory of the spin-galvanic effect and the anomalous phase shift  $\varphi_0$  in superconductors and Josephson junctions with intrinsic spin-orbit coupling  
Physical Review B 92, 125443 (2015).



**Figure:** (a) Scanning electron microscopy image of the active region of the phase battery composed by the two  $\varphi_0$ -junctions.  $B_y$  is the in-plane magnetic field orthogonal to the nanowire. (b) Sketch of the interferometer with the reference axes of the in-plane magnetic field ( $B_{in}$ ) and the angle  $\theta$  with respect to the nanowire axis. (c) Dependence of the extrinsic anomalous phase  $\varphi_{ex}$  on  $B_y$ . It results in an odd symmetry and non-hysteretic back and forth sweeps (blue and red traces). Inset: the  $\varphi_{ex}(B_y)$  dependence obtained from our theoretical model. (d) Plot of  $\partial\varphi_{ex}/\partial B_{in}$  versus  $\theta$  together with a theoretical fit (red curve).

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

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

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

Nature Communications 11, 1124 (2020)

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

The four scientists examined germanium selenide (GeSe), a material with a rectangular unit cell, rather than focusing on lattices with three- or six-fold symmetries like graphene or  $\text{WSe}_2$ . By combining large scale ab-initio and density matrix renormalization group calculations, the researchers showed that the Moiré interference pattern creates parallel wires of correlated one-dimensional systems.

This considerably broadens the scope for realizable structures using Moiré twisting physics and provides an inroad into the challenging question of how a correlated system crosses over from two dimensions to one. Because the particles cannot pass each other as they

would in a multi-dimensional context, one-dimensional systems are intriguing, as correlations necessarily lead to collective excitations.

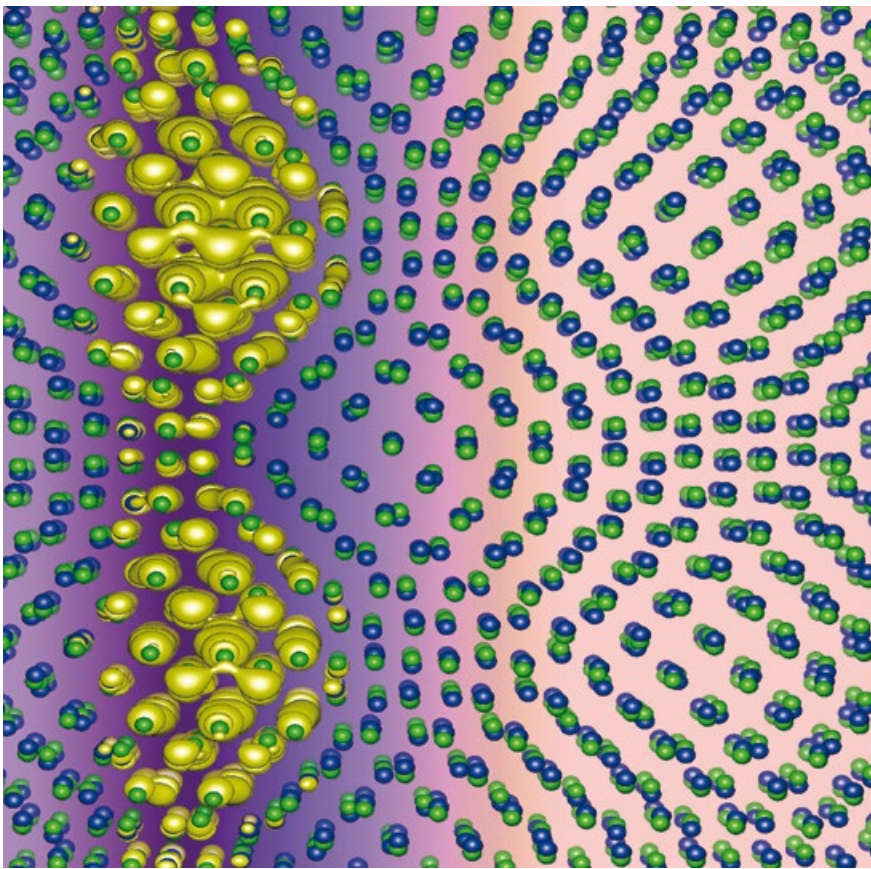
Dante Kennes says the combined analysis of the two numerical methods yielded great results: “We were able to classify the phase diagram of two sheets of twisted GeSe and found a plethora of realizable phases of matter, including correlated Mott insulators and the so-called Luttinger liquid phase, which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

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

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

fundamental computational building block.

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



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

# Directional shift current in mirror-symmetric $BC_2N$

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

Physical Review Research 2, 13263 (2020)

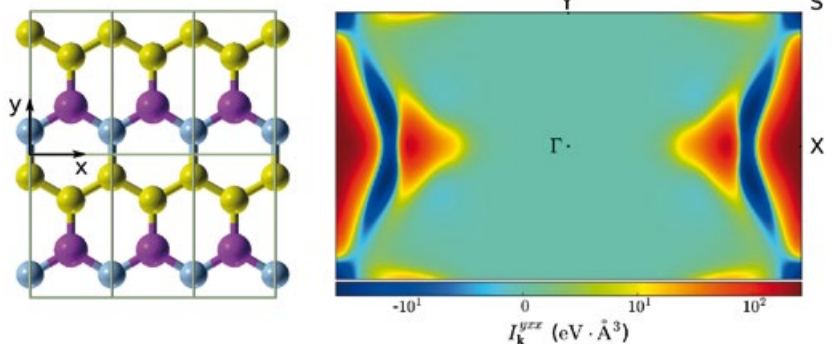
Ibanez-Azpiroz et al. theoretically describe the shift-current photoconductivity of graphitic  $BC_2N$ . It is strongly anisotropic near the fundamental gap due to quantum dipole selection rules imposed by mirror symmetry, which imply that the relative parities between valence and conduction bands are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

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

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

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

“Dipole selection rules determine the nonlinear response to light of graphitic  $BC_2N$ ”



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

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

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

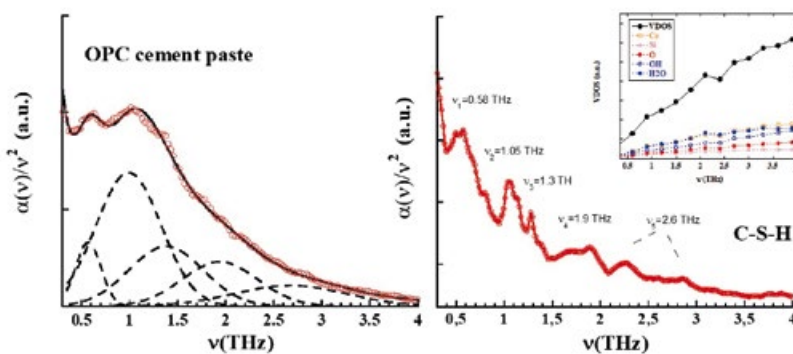
Materials 13, 4194 (2020)

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

Cementitious materials contain many structural features that seem to favour the response to the THz radiation. On the one hand, their local structure is glassy and amorphous, something which is known to give rise to an overpopulation of vibrational states at the THz frequencies, the so-called Boson Peaks. On the other hand, they contain plenty of water molecules that strongly interact with light due to their intrinsic electric dipole.

Besides, the nanoporous skeleton of cement-based materials provides a rich topology for investigating the intrinsic Bosonic states of water, often studied in super-cooled or nanoconfined water.

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



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



## 13

# Atomic-scale dissection of molecular flashes

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

Nature Nanotechnology 15, 207 (2020)

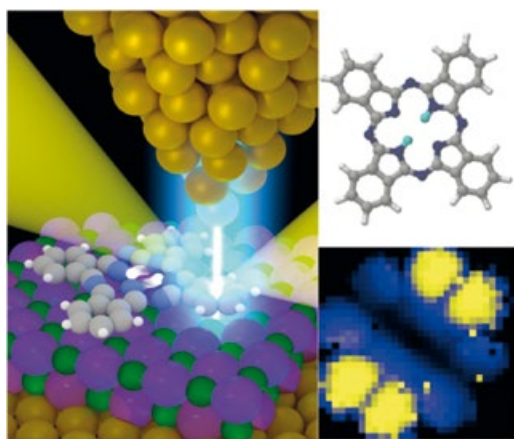
Molecules are key building blocks for future optoelectronic devices at extremely low dimensions, as they can carry electronic current, emit photons, or switch on and off a signal. Thanks to an ultra-resolved nanoscopy technique, it is now possible to map the origin of light emitted from a switching molecule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

Single-molecule devices open up functionalities that go beyond today's electronics due to their intrinsic quantum nature. The concept of single molecule optoelectronics, which consists in combining optical and electronic properties within a single molecule, strongly emerges in this context. In molecular optoelectronics it is envisioned that light could be used to convey information at high frequen-

cy between well-separated components (atoms) within a single-molecule. This objective to access the molecular internal structure and its dynamics is closer thanks to the achievement by researchers at IPCMS of Strasbourg. These researchers implemented a nanoscopic technique which allowed to distinguish the exact origin of a molecular flash inside a molecule at the atomic scale. The team of researchers observed an unexpected blinking of the emitted light from the molecule, and together with theoretician colleagues from the "Theory of Nanophotonics" group at CFM in San Sebastian, they identified and associated the molecule's flash fluctuation to the switching of hydrogen atoms between two positions of the molecule (about 1000 times per second), in a mechanism known as tautomerization. This result provides new information on this reaction, and shows that a molecule may be used as an intermittent emitter, potentially controllable, and relevant for optical communications at the nanoscale.

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

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



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

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

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

Nanoscale 12, 16875 (2020)

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

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

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

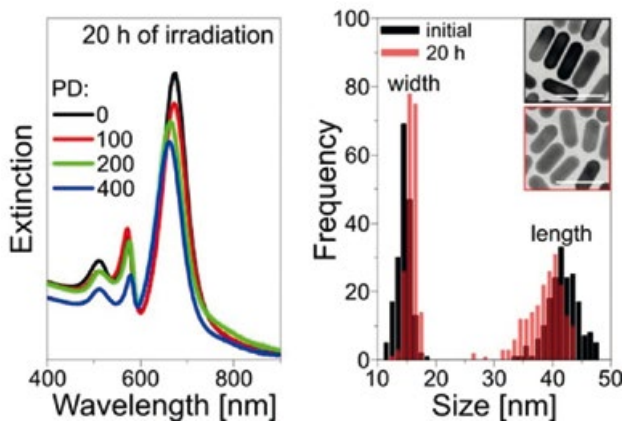
The present work shows that nano hybrid systems, composed of plasmonic nanoparticles and J-aggregates of organic molecules, display outstanding resistance to harsh environmental stressors such as temperature, pH and strong light irradiation as well as demonstrate long-term stability and processability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

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

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

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



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

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

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

Optical Materials Express 10, 2695 (2020)

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

The use of ultrashort laser pulses for the inscription of optical waveguides in transparent dielectrics has attracted great attention since the first demonstration due to the intrinsic properties of the technique; the fabrication is direct and can be applied to almost any transparent dielectric, it does not require any specific sample preparation and, more remarkably, it allows the implementation of 3D structures. Among the different substrates used for waveguide inscription by femto-

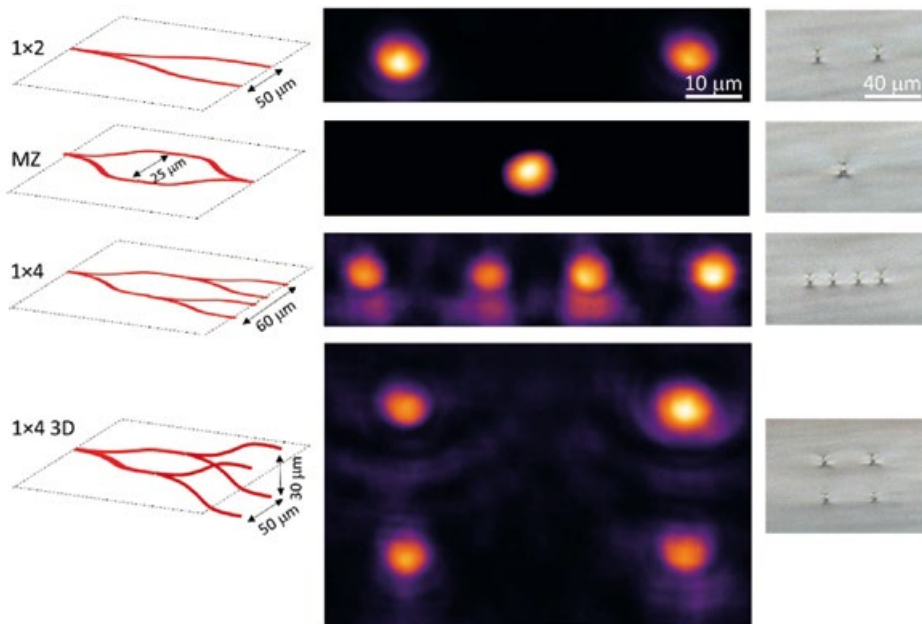
second laser irradiation, oxyfluoride nano-glass ceramics containing rare-earth doped fluoride nanocrystals combine the good mechanical and chemical stabilities of oxide glasses with the low phonon energy of fluoride crystals, thus being of great interest in the operation of active devices.

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

The suitability of the glass-ceramics as substrate for the integration of complex photonic elements was demon-

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



**Figure:** Scheme of the implemented photonic elements (left column), normalized near-field modal profiles at 800 nm (central column), and microscopic pictures of the output facet (right column). From top to bottom, 1x2 splitter, Mach-Zehnder interferometer, 1x4 splitter (2D), and 1x4 splitter (3D).

## 16

# Kerker conditions upon lossless, absorption, and optical gain regimes

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

Physical Review Letters 125, 073205 (2020)

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

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

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

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

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

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

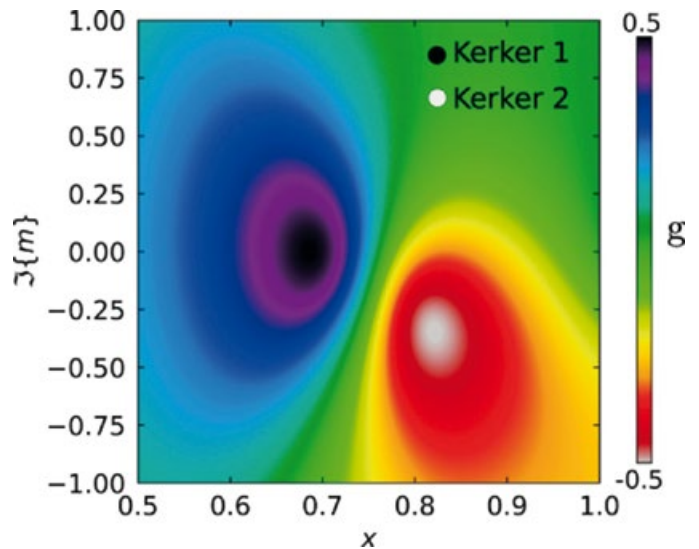
For a germanium (Ge) sphere in the dipolar regime, the team quantifies the gradual drift from the ideal zero optical backscattering condition as the absorption rate is increased. Finally, that optical gain is mandatory to reach the zero forward light scattering condition is demonstrated.

The researchers show that the electromagnetic helicity cannot be preserved after scattering by an arbitrary dielectric sphere in the presence of losses or optical gain.

Hence, neither can the zero optical backscattering condition be fulfilled in that scenario.

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

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



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

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

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

Physical Review Research 2, 022015 (2020)

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

The collective dynamics of water in the terahertz range has been intensively investigated since the 1970's. Most studies used Inelastic X-ray Scattering (IXS), and invoked a viscoelastic model that assumes the existence of a "structural" relaxation process. A direct observation by IXS of this relaxation is, however, difficult

due to the current resolution of IXS. IXS is also usually limited to mesoscopic scales (scattering vector  $0.2 \leq Q \leq 0.7 \text{ \AA}^{-1}$ ). Thus, the crossover towards the inter-molecular scale ( $Q \approx 2 \text{ \AA}^{-1}$  for water) had not been well explored up to now.

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

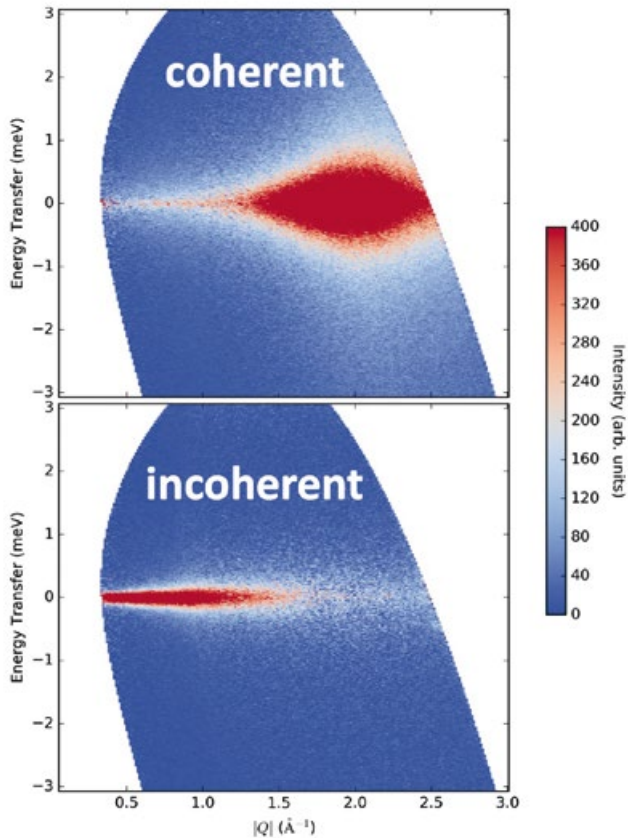
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the convolution of a Q-independent mode and diffusion. The combination with Molecular Dynamics simulations carried out at the Materials Physics Centre was very helpful for the data interpretation.

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

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



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

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# Direct observation of desorption of a melt of long polymer chains

**Monnier X, Napolitano S, and Cangialosi D.**

Nature Communications 7, 2292 (2020)

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

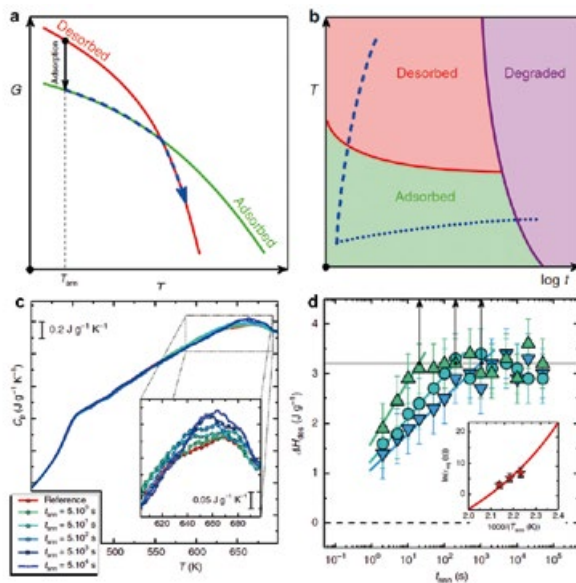
The concomitant decrease of enthalpy and entropy in adsorption is analogous to the well-known phenomenon of crystallization. Within this analogy, increasing the temperature entails the progressive enhancement of the entropic part of the free energy and, thereby, the opposite phenomenon – that is, desorption,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

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

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

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

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



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

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

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

Materials Horizons 7, 2292 (2020) - REVIEW

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

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

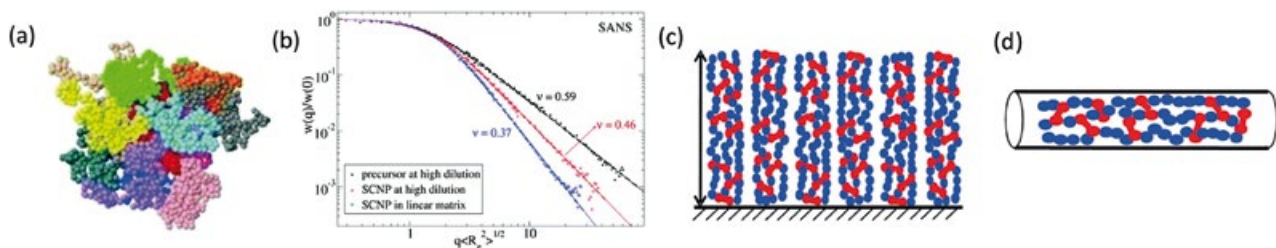
Self-confinement in SCNPs has already been exploited for catalysis, encapsulation, transport and delivery of therapeutic cargos, sensing, targeting and bioimaging applications, as well as a variety of other advanced applications. Further progress is expected in these fields accompanied by the development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

presumably lead to precise control of the SCNP topology and, hence, to highly accurate structure–property relationships.

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

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

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

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

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# The instrument suite of the European Spallation Source (ESS)

ESS Collaboration, including Fernandez-Alonso F.

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

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

The instrument suite described in this work represents the culmination of continued efforts across a wide range of disciplines and institutions over the past decade. The ESS is an accelerator-based, pulsed-neutron source optimized to provide high flux, flexible resolution, and broad bandwidth, capabilities that translate into a plethora of new scientific opportunities. A total of fifteen instruments have been designed to this end, with a view to their imminent construction and subsequent deployment: two small-angle scattering instruments and two reflectometers; an imaging station; five diffractometers

for the study of single crystals, macromolecular systems, magnetism, and engineering; and five inelastic neutron spectrometers spanning a wide range of length- and time scales simultaneously – one of the primary merits and strengths of neutron-scattering techniques, as illustrated in the accompanying figure. The team at the Materials Physics Center has been particularly focused on the VESPA spectrometer, including its science case and specification. This task has benefitted greatly from recent and joint developments at other neutron sources worldwide, most notably on TOSCA at the ISIS Pulsed Neutron & Muon Source in the United Kingdom. Both VESPA and TOSCA are high-resolution broadband spectrometers ideally suited to explore the properties of new materials, from fuel stores and nanostructured media to supramolecular frameworks for carbon-dioxide capture. On VESPA, the variable spectral resolution coupled to simultaneous diffraction also paves the way for parametric and kinetic studies that would offer an unprecedented level of detail and insight currently beyond our reach.

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

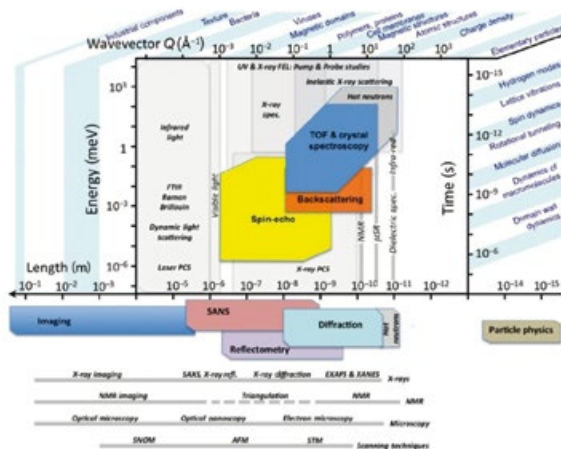
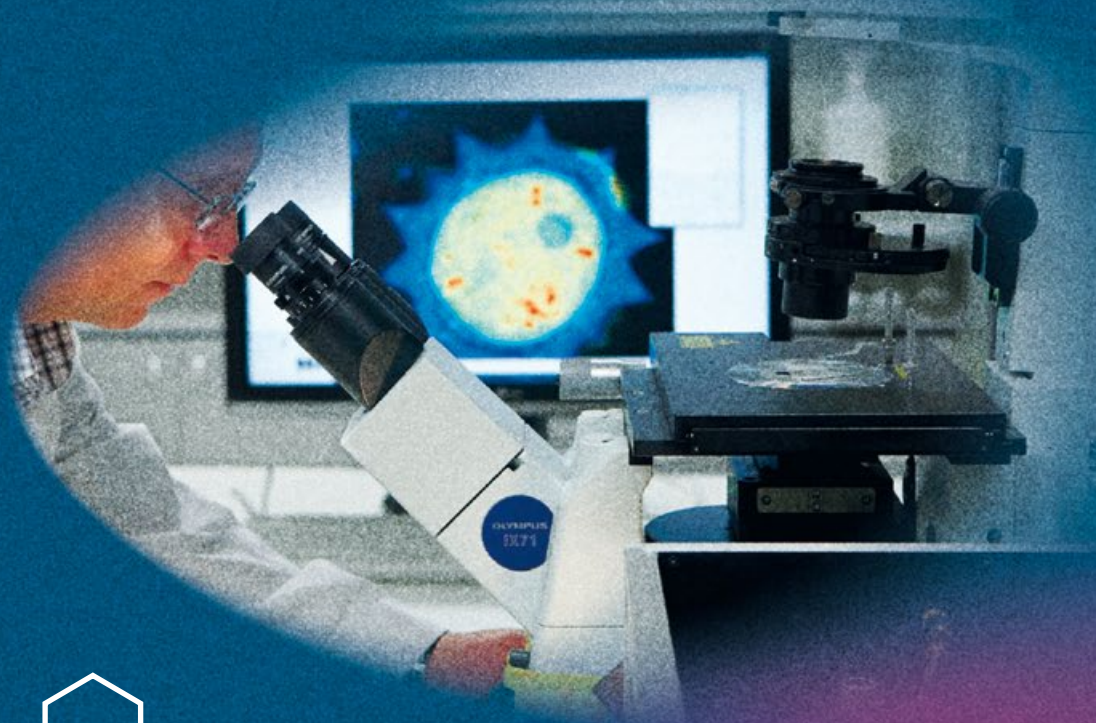


Figure: Length and time scales accessible to neutrons, along with a qualitative comparison with other experimental probes. Adapted from Fernandez-Alonso F and Price DL, Neutron Scattering – Fundamentals (Academic Press, 2013).

# FACILITIES & EXTERNAL SERVICES

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



# FACILITIES

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

## CHEMICAL PHYSICS OF COMPLEX MATERIALS

### HIGH RESOLUTION ANGLE RESOLVED PHOTOEMISSION LAB

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

### SURFACE CHEMICAL-PHYSICS LAB

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

### SURFACE MAGNETISM LAB

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

### ULTRA-LOW TEMPERATURE SCANNING TUNNELING MICROSCOPY LAB

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

## ELECTRONIC PROPERTIES AT THE NANOSCALE

### CERAMICS AND CEMENT-BASED MATERIALS LAB

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

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

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



## PHOTONICS

### LASER SPECTROSCOPY LAB

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

### ULTRAFAST SPECTROSCOPY LAB

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

### NANOPHOTONICS LAB

The “Nanophotonics” laboratory hosts a scanning confocal time-resolved photoluminescence (TRPL) microscopy setup (MicroTime200, PicoQuant) with single molecule detection sensitivity, equipped with two lasers (405 and 485 nm), two single-photon counting avalanche photodetectors, heating stage, and cryostat. The system contains the complete optics and electronics for recording all main aspects of the luminescence dynamics down to single nanoparticle / molecule level with wide range of capabilities: 2D and

3D Confocal photoluminescence microscopy imaging o Single molecule imaging; 2D and 3D Fluorescence Lifetime Imaging (FLIM); the minor carriers lifetime mapping; carriers recombination dynamics; and Forster Resonance Energy Transfer (FRET).

Other available set-ups include:

- QUEPRO high-performance spectrophotometer connected to IX71 Olympus microscope for micro-photoluminescence spectroscopy
- MayaPro2000 spectrophotometer (Ocean Optics)
- Cary50 spectrophotometer (Agilent) for absorption and transmission spectroscopy
- Cary 3500 (Agilent) with kinetics and temperature control
- Cary Eclipse Spectrophotometers (Agilent) for range of applications including photoluminescence and photoluminescence excitation spectroscopy, photoluminescence anisotropy spectroscopy, photoluminescence kinetics, phosphorescence and delayed fluorescence lifetime measurements
- Chemat KW4A precision spin-coater for deposition of thin organic and inorganic films from solutions and self-assembly of nanostructures
- Thermal cycler (Applied Biosystems) for 96 wells
- Two programmable syringe pumps (WPI) operating at wide range of flow rates
- Two illumination sources of 150 W quartz halogen fiber optic illuminator (Dolan- Jenner) equipped with the set of bandpass and long-pass filter (Edmund Optics, and Intor)
- Portable photometer equipped with global radiometer sensor (400 – 2000 nm)
- Oxygen sensor (Neo Fox, Ocean Optics)
- Thermocouples operating in wide range of temperatures and solvents (ThorsLab)

# FACILITIES

## MATERIALS SYNTHESIS LAB

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

## QUANTUM NANOPHOTONICS LAB

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

- Three optical tables for manipulating the polarisation as well as spatial and frequency degrees of freedom of entangled and single photon states: 1200 x 2400 x 305 mm table with isolators (784-655-12DR model from TMC), 1500 x 3000 x 305 mm table with isolators (784-675-12DR model from TMC) and 900 mm x 1800 mm x 305 mm table with isolators (from Newport)
- A set of laser systems, including continuous wave lasers covering the ultra violet, visible and infrared regions, for producing different photon states: a 633nm, 10mW, He-Ne laser (from Thorlabs); an 403nm, 100mW, diode (from Toptica); a 680nm, 50mW, diode (from Toptica); an 808nm, 10mW, diode (from Thorlabs)
- A source of entangled photons based on a periodically poled potassium titanyl phosphate (ppKTP) crystal
- Optically addressable cryostat, equipped with state-of-the-art nanopositioners, for cooling down nanostructures and nanoparticles to cryogenic temperatures (attoDRY 100 model from Attocube)
- A set of spatial light modulators (from Cambridge Correlators), polarisers (from Thorlabs and Standa) and Single Photon Counting Modules (SPCM, APDs SPCM-AQ4C model from Excelitas), for analysing the photons interacting with nanostructures at cryogenic temperatures

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

## POLYMERS AND SOFT MATTER

## DIELECTRIC SPECTROSCOPY LAB

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

- Broad-Band Dielectric Spectrometers (BBDS): ALPHA-S & ALPHA-A Novocontrol
- High-Frequency Dielectric Spectrometer (HFDS): Agilent E4991A RF-Impedance Analyzer
- Micro-Wave Dielectric Spectrometer (MWDS): Agilent E8361A Microwave Network Analyzer
- Terahertz Spectrometer (THS): Teraview 3000 spectrometer
- High-Pressure Dielectric Spectrometer (HPDS): Concept 100 Novocontrol
- Low-Temperature Dielectric spectrometer (LTDS): ALPHA-A Novocontrol
- Time-Domain Dielectric Spectrometer (TDDS): Novocontrol
- Thermally Stimulated Depolarisation Currents (TSDC): Novocontrol

## MICROSCOPY LAB

The "Microscopy" laboratory allows materials structural characterisation by means of:

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

## CHEMISTRY LAB

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

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

## THERMAL CHARACTERISATION LAB

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

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

## REOLOGICAL CHARACTERISATION LAB

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

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

## ABSORPTION SPECTROSCOPY TECHNIQUES LAB

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

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

# FACILITIES

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## X-RAY LAB

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

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

## LIGHT SCATTERING LAB

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

## HIGH PERFORMANCE COMPUTING (HPC) CENTRE

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

There are currently four CFM HPC clusters:

- **Oberon** cluster (the main, general purpose, CFM HPC cluster), composed of 182 computing nodes with two Xeon processors and a memory range of 24 GB up to 256 GB per node, all of them sharing a high speed-low latency Infiniband connection network and a high performance shared parallel filesystem, giving a total of 2000 cores and 15 TB of memory. This cluster gives service to the whole CFM research community.
- **Nostramo** cluster, targeted to shared memory – single node molecular dynamics calculations. It is composed of 17 AMD Opteron 6300 series computing nodes with 64 cores and 64 GB of RAM each node, giving a total of 1088 cores and about 1.1 TB of memory.
- **Ekhi** cluster, designed specifically for novel Quantum ESPRESSO calculations, is composed of 28 computing nodes with two Xeon Cascade Lake-SP 6230 processors (40 computing cores) and 96 GB of memory in each node, with an Infiniband FDR interconnection network, giving a total of 1120 cores and 2.7 TB of memory.
- **Sama** is a multipurpose cluster designed for high-level ab initio electronic structure calculations and molecular dynamics simulations. It is composed of 13 computing nodes with two Intel Xeon Gold 6240R processors (48 cores), 384 GB of memory, and 1 TB NVMe SSD disk per node, all interconnected through an Infiniband HDR 100 Gb/s network, and giving a total of 624 cores and 4.8TB of memory.

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

# EXTERNAL SERVICES

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

## DIFFERENTIAL THERMAL ANALYSIS (DTA)

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

## ISOBARIC THERMAL EXPANSION

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

## ABSORPTION SPECTROSCOPY IN TERAHERTZ (THZ) DOMAIN

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

## DIELECTRIC CHARACTERISATION

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

## SMALL-ANGLE X-RAY DIFFRACTION

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

## MATERIALS SURFACE CHARACTERISATION

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

## NANOPHOTONICS LAB

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

## HIGH PERFORMANCE COMPUTING (HPC) SUPPORT

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

# RESEARCH OUTPUT

Among all the articles published at CFM, **81 %** were published in the framework of **international collaborations**, showing the international dimension and positioning of the Centre in the field of Materials Science.

ISI Publications

217

Q1 Publications

142

D1 Publications

89

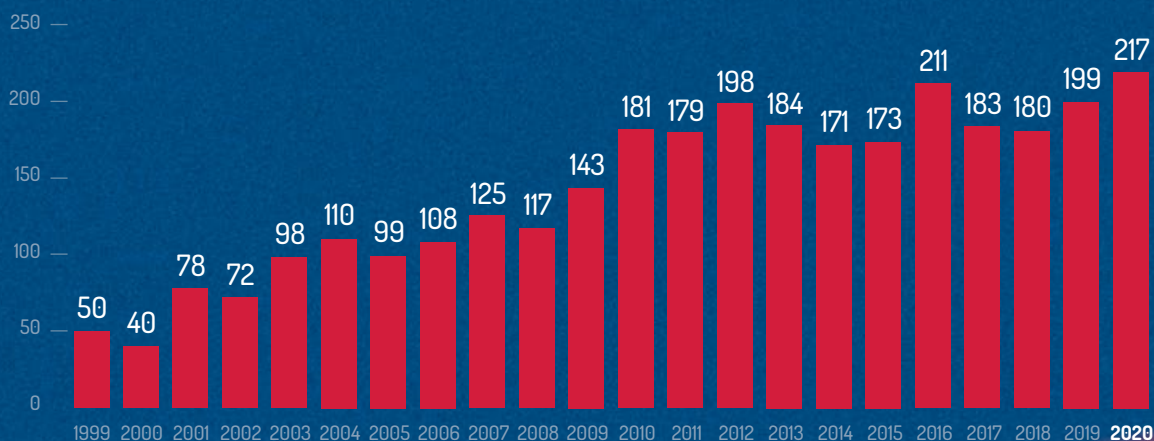
H-Index

133

ISI Web of Science citations

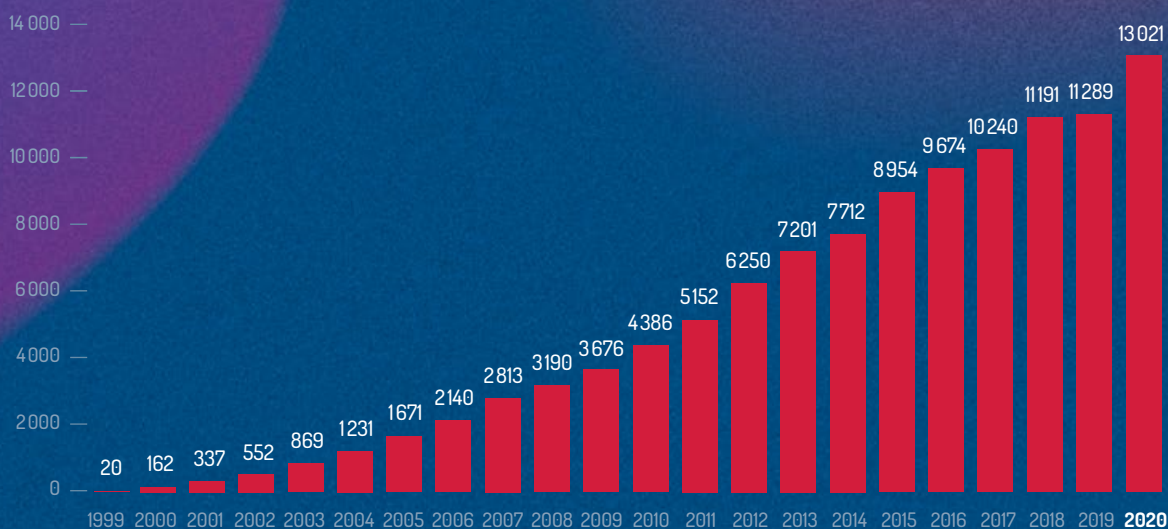
13 021\* in 2020  
\*As of April 2021

# PUBLICATIONS



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

# CITATIONS



Total number of ISI citations since 1999: **117718**  
H index as of April 2021: **133**

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

62

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



# PUBLICATIONS

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## **1 Theory of the thickness dependence of the charge density wave transition in 1 T-TiTe<sub>2</sub>**

Zhou JS, Bianco R, Monacelli L, Errea I, Mauri F, and Calandra M.  
2D Materials 7, 45032 (2020)

## **2 Cellulose as an inert scaffold in plasmon-assisted photoregeneration of cofactor molecules**

Tarnowicz-Staniak N, Vazquez-Diaz S, Pavlov V, Matczyszyn K, and Grzelczak M.  
ACS Applied Materials & Interfaces 12, 19377 (2020)

## **3 Kinetic and thermodynamic hysteresis in clustering of gold nanoparticles: Implications for nanotransducers and information storage in dynamic systems**

Kruse J, Merkens S, Chuvilin A, and Grzelczak M.  
ACS Applied Nano Materials 3, 9520 (2020)

## **4 Ultrafast real-time dynamics of CO oxidation over an oxide photocatalyst**

Wagstaffe M, Wenthaus L, Dominguez-Castro A, Chung SM, Semione GD, Palutke S, Mercurio G, Dziarzhyski S, Redlin H, Klemke N, Yang YD, Frauenheim T, Dominguez A, Kartner F, Rubio A, Wurth W, Stierle A, and Noei H.  
ACS Catalysis 10, 13650 (2020)

## **5 Resolving segmental polymer dynamics in nanocomposites by incoherent neutron spin-echo spectroscopy**

Musino D, Oberdisse J, Farago B, Alegria A, and Genix AC.  
ACS Macro Letters 9, 910 (2020)

## **6 Cyclic polyethylene glycol as nanoparticle surface ligand**

Aboudzadeh MA, Iturrospe A, Arbe A, Grzelczak M, and Barroso-Bujans F.  
ACS Macro Letters 9, 1604 (2020)

## **7 Present and future of surface-enhanced Raman scattering**

Langer J, de Aberasturi DJ, Aizpurua J, Alvarez-Puebla RA, Auguie B, Baumberg JJ, Bazan GC, Bell SEJ, Boisen A, Brolo AG, Choo J, Ciolla-May D, Deckert V, Fabris L, Faulds K, de Abajo FJG, Goodacre R, Graham D, Haes AJ, Haynes CL, Huck C, Itoh T, Ka M, Kneipp J, Kotov NA, Kuang H, Le Ru EC, Lee HK, Li JF, Ling XY, Maier SA, Mayerhofer T, Moskovits M, Murakoshi K, Nam JM, Nie S, Ozaki Y, Pastoriza-Santos I, Perez-Juste J, Popp J, Pucci A, Reich S, Ren B, Schatz GC, Shegai T, Schlucker S, Tay LL, Thomas KG, Tian ZQ, Van Duyne RP, Vo-Dinh T, Wang Y, Willets KA, Xu C, Xu H, Xu Y, Yamamoto YS, Zhao B, and Liz-Marzan LM.  
ACS Nano 14, 28 (2020)

## **8 Band depopulation of graphene nanoribbons induced by chemical gating with amino groups**

Li JC, Brandimarte P, Vilas-Varela M, Merino-Diez N, Moreno C, Mugarza A, Mollejo JS, Sanchez-Portal D, de Oteyza DG, Corso M, Garcia-Lekue A, Pena D, and Pascual JI.  
ACS Nano 14, 1895 (2020)

## **9 Single photon emission from a plasmonic light source driven by a local field-induced coulomb blockade**

Leon CC, Gunnarsson O, de Oteyza DG, Roslawska A, Merino P, Grewal A, Kuhnke K, and Kern K.  
ACS Nano 14, 4216 (2020)

## **10 Probing the magnetism of topological end states in 5-armchair graphene nanoribbons**

Lawrence J, Brandimarte P, Berdonces-Layunta A, Mohammed MSG, Grewal A, Leon CC, Sanchez-Portal D, and de Oteyza, DG.  
ACS Nano 14, 4499 (2020)

## **11 Molecular approach for engineering interfacial interactions in magnetic/topological insulator heterostructures**

Cuxart MG, Valbuena MA, Robles R, Moreno C, Bonell F, Sauthier G, Imaz I, Xu H, Nistor C, Barla A, Gargiani P, Valvidares M, MasPOCH D, Gambardella P, Valenzuela SO, and Mugarza A.  
ACS Nano 14, 6285 (2020)

## **12 Multiscale analysis of phase transformations in self-assembled layers of 4,4'-Biphenyl dicarboxylic acid on the Ag(001) Surface**

Prochazka P, Gosalvez MA, Kormos L, de la Torre B, Gallardo A, Alberdi-Rodriguez J, Chutora T, Makoveev AO, Shahsavari A, Arnau A, Jelinek P, and Cechal J.  
ACS Nano 14, 7269 (2020)

## **13 Topologically nontrivial phase-change compound GeSb<sub>2</sub>Te<sub>4</sub>**

Nurmamat M, Okamoto K, Zhu SY, Menshchikova TV, Rusinov IP, Korostelev VO, Miyamoto K, Okuda T, Miyashita T, Wang XX, Ishida Y, Sumida K, Schwier EF, Ye M, Aliev ZS, Babanly MB, Amiraslanov IR, Chulkov EV, Kokh KA, Tereshchenko OE, Shimada K, Shin S, and Kimura A.  
ACS Nano 14, 9059 (2020)

## **14 Effect of paclitaxel in the water dynamics of MCF-7 breast cancer cells revealed by dielectric spectroscopy**

Martins ML, Bordallo HN, Arrese-Igor S, Alegria A, and de Leon JC.  
ACS Omega 5, 18602 (2020)

## **15 Second-harmonic generation from a quantum emitter coupled to a metallic nanoantenna**

Babaze A, Esteban R, Aizpurua J, and Borisov AG.  
ACS Photonics 7, 701 (2020)

## **16 Probing the radiative electromagnetic local density of states in nanostructures with a scanning tunneling microscope**

Cao SY, Zapata-Herrera M, Campos A, Le Moal E, Marguet S, Dujardin G, Kociak M, Aizpurua J, Borisov A, and Boer-Duchemin E.  
ACS Photonics 7, 1280 (2020)

## **17 The crystal field plasmon splitting**

Mezzasalma SA, Grzelczak M, and Sancho-Parramon J.  
ACS Photonics 7, 1551 (2020)

## **18 Optomechanical collective effects in surface-enhanced Raman scattering from many molecules**

Zhang Y, Aizpurua J, and Esteban R.  
ACS Photonics 7, 1676 (2020)

## **19 Surface-enhanced circular dichroism spectroscopy on periodic dual nanostructures**

Lasa-Alonso J, Abujetas DR, Nodar A, Dionne JA, Saenz JJ, Molina-Terriza G, Aizpurua J, and Garcia-Etxarri A.  
ACS Photonics 7, 2978 (2020)

## **20 Terahertz nanoimaging and nanospectroscopy of chalcogenide phase-change materials**

Chen C, Chen S, Lobo RPSM, Maciel-Escudero C, Lewin M, Taubner T, Xiong W, Xu M, Zhang XL, Miao XS, Li PN, and Hillenbrand R.  
ACS Photonics 7, 5499 (2020)

# PUBLICATIONS

---

## **21 Relevance of the quadratic diamagnetic and self-polarization terms in cavity quantum electrodynamics**

Schafer C, Ruggenthaler M, Rokaj V, and Rubio A.  
ACS Photonics 7, 975 (2020)

## **22 Infrared permittivity of the biaxial Van der Waals semiconductor $\alpha$ - $\text{MoO}_3$ from near- and far-field correlative studies**

Alvarez-Perez G, Foland TG, Errea I, Taboada-Gutierrez J, Duan JH, Martin-Sanchez J, Tresguerres-Mata AIF, Matson JR, Bylinkin A, He MZ, Ma WL, Bao QL, Martin JI, Caldwell JD, Nikitin AY, and Alonso-Gonzalez P.  
Advanced Materials 32, 1908176 (2020)

## **23 The importance of quantifying the composition of the amorphous intermixed phase in organic solar cells**

Marina S, Kaufmann NP, Karki A, Gutierrez-Meza E, Gutierrez-Fernandez E, Vollbrecht J, Solano E, Walker B, Bannock JH, de Mello J, Silva C, Nguyen TQ, Cangialosi D, Stingelin N, and Martin J.  
Advanced Materials 32, 2005241 (2020)

## **24 Recent advances in solid-state lighting devices using transition metal complexes exhibiting thermally activated delayed fluorescent emission mechanism**

Mahoro GU, Fernandez-Cestau J, Renaud JL, Coto PB, Costa RD, and Gaillard S.  
Advanced Optical Materials 8, 2000260 (2020)

## **25 Enhanced light-matter interaction in B-10 monoisotopic boron nitride infrared nanoresonators**

Autore M, Dolado I, Li PN, Esteban R, Alfaro-Mozaz FJ, Atxabal A, Liu S, Edgar JH, Velez S, Casanova F, Hueso LE, Aizpurua J, and Hillenbrand R.  
Advanced Optical Materials, 2001958 (2020) (Early Access)

## **26 Probing the network topology in network-forming materials: The case of water**

Formanek M, and Martelli F.  
AIP Advances 10, 55205 (2020)

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

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

## **28 Electrochemical stability of the reconstructed $\text{Fe}_3\text{O}_4(001)$ surface**

Grumelli D, Wiegmann T, Barja S, Reikowski F, Maroun F, Allongue P, Balajka J, Parkinson GS, Diebold U, Kern K, and Magnussen OM.  
Angewandte Chemie-International Edition (Early Access)

## **29 Controlling single molecule conductance by a locally induced chemical reaction on individual thiophene units**

Michnowicz T, Borca B, Petuya R, Schendel V, Pristl M, Pentegov I, Kraft U, Klauk H, Wahl P, Mutombo P, Jelinek P, Arnau A, Schlickum U, and Kern K.  
Angewandte Chemie-International Edition 59, 6207 (2020)

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

Barragan A, Sarasola A, and Vitali L.  
Angewandte Chemie-International Edition 59, 15599 (2020)

# PUBLICATIONS

---

## **31 Catalytic oxidation of CO on a curved Pt(111) surface: simultaneous ignition at all facets through a transient CO-O complex**

Garcia-Martinez F, Garcia-Fernandez C, Simonovis JP, Hunt A, Walter A, Waluyo I, Bertram F, Merte LR, Shipilin M, Pfaff S, Blomberg S, Zetterberg J, Gustafson J, Lundgren E, Sanchez-Portal D, Schiller F, and Ortega JE. *Angewandte Chemie-International Edition* 59, 20037 (2020)

## **32 Effect of spectral overlap and separation distance on exciton and biexciton quantum yields and radiative and nonradiative recombination rates in quantum dots near plasmon nanoparticles**

Krivenkov V, Dyagileva D, Samokhvalov P, Nabiev I, and Rakovich Y. *Annalen der Physics* 523, 2000236 (2020)

## **33 Superconducting hydrides under pressure**

Pickard CJ, Errea I, and Eremets MI. *Annual Review of Condensed Matter Physics* 11, 57 (2020)

## **34 Signatures of temperature driven antiferromagnetic transition in the electronic structure of topological insulator $\text{MnBi}_2\text{Te}_4$**

Estyunin DA, Klimovskikh II, Shikin AM, Schwier EF, Otrokov MM, Kimura A, Kumar S, Filnov SO, Aliev ZS, Babanly MB, and Chulkov EV. *APL Materials* 8, 21105 (2020)

## **35 Quantification of interfacial spin-charge conversion in hybrid devices with a metal/insulator interface**

Sanz-Fernandez C, Pham VT, Sagasta E, Hueso LE, Tokatly IV, Casanova F, and Bergeret FS. *Applied Physics Letters* 117, 142405 (2020)

## **36 Very large thermal rectification in ferromagnetic insulator-based superconducting tunnel junctions**

Giazotto F, and Bergeret FS. *Applied Physics Letters* 116, 192601 (2020)

## **37 Using gold nanoparticles to detect single-nucleotide polymorphisms: toward liquid biopsy**

Iglesias MS, and Grzelczak M. *Beilstein Journal of Nanotechnology* 11, 263 (2020)

## **38 Human importin alpha 3 and its N-terminal truncated form, without the importin-beta-binding domain, are oligomeric species with a low conformational stability in solution**

Diaz-Garcia C, Hornos F, Giudici AM, Camara-Artigas A, Luque-Ortega JR, Arbe A, Rizzuti B, Alfonso C, Forwood JK, Iovanna JL, Gomez J, Prieto M, Coutinho A, and Neira JL. *Biochimica et Biophysica Acta-General Subjects* 1864, 129609 (2020)

## **39 Keto-enol tautomerization drives the self-assembly of leucoquinizarin on Au(111)**

Costantini R, Colazzo L, Batini L, Stredansky M, Mohammed MSG, Achilli S, Floreano L, Fratesi G, de Oteyza DG, and Cossaro A. *Chemical Communications* 56, 2833 (2020)

## **40 Steering alkyne homocoupling with on-surface synthesized metal-organic complexes**

Mohammed MSG, Colazzo L, Gallardo A, Pomposo JA, Jelinek P, and de Oteyza DG. *Chemical Communications* 56, 8659 (2020)

**41 Microwave irradiation versus conventional heating assisted free-radical copolymerization in solution**

Perez-Martinez BT, Aboudzadeh MA, Schubert US, Leiza JR, and Tomovska R.  
Chemical Engineering Journal 399, 125761 (2020)

**42 Modelling the dynamic development of the curing process and film morphology of films cast from waterborne acrylic-alkyd hybrids**

Limousin E, Gonzalez E, Martinez-Tong DE, Ballard N, and Asua JM.  
Chemical Engineering Journal 400, 125891 (2020)

**43 Transferring axial molecular chirality through a sequence of on-surface reactions**

Merino-Diez N, Mohammed MSG, Castro-Esteban J, Colazzo L, Berdonces-Layunta A, Lawrence J, Pascual JI, de Oteyza DG, and Pena D.  
Chemical Science 11, 5441 (2020)

**44 Smart microgels as drug delivery vehicles for the natural drug aescin: uptake, release and interactions**

Dirksen M, Dargel C, Meier L, Brandel T, and Hellweg T.  
Colloid and Polymer Science 298, 5050 (2020)

**45 Electronic and magnetic characterization of epitaxial  $VSe_2$  monolayers on superconducting  $NbSe_2$**

Kezilebieke S, Huda MN, Dreher P, Manninen I, Zhou YF, Sainio J, Mansell R, Ugeda MM, van Dijken S, Komsa HP, and Liljeroth P.  
Communications Physics 3, 116 (2020)

**46 Electronic decoupling of polyacenes from the underlying metal substrate by  $sp^3$  carbon atoms**

Mohammed MSG, Colazzo L, Robles R, Dorel R, Echavarren AM, Lorente N, and de Oteyza DG.  
Communications Physics 3, 159 (2020)

**47 Thermally induced structural transitions between single-crystalline states in the first hybrid compound combining Keggin-type clusters with metal-cyclam complexes: From two-dimensional covalent assemblies to discrete molecular species**

Fernandez-Navarro L, Iturrospe A, Reinoso S, Artetxe B, Ruiz-Bilbao E, San Felices L, and Gutierrez-Zorrilla JM.  
Crystal Growth & Design 20, 3499 (2020)

**48 Effect of Cr on the hydrogen storage and electronic properties of BCC alloys: Experimental and first-principles study**

Balcerzak M, Wagstaffe M, Robles R, and Pruneda M.  
International Journal of Hydrogen Energy 45, 28996 (2020)

**49 Melts of single-chain nanoparticles: A neutron scattering investigation**

Arbe A, Rubio J, de Molina PM, Maiz J, Pomposo JA, Fouquet P, Prevost S, Juranyi F, Khanefit M, and Colmenero J.  
Journal of Applied Physics 127, 44305 (2020)

**50 Chemical and structural heterogeneities in Nd-doped oxynitride phosphate laser glasses**

Munoz F, Jimenez-Rioboo RJ, and Balda R.  
Journal of Alloys and Compounds 816, 152657 (2020)

## **51 Tuning paramagnetic effect of Co-doped CdS diluted magnetic semiconductor quantum dots**

Ibraheem F, Mahdy MA, Mahmoud EA, Ortega JE, Rogero C, Mahdy IA, and El-Sayed A.  
Journal of Alloys and Compounds 834, 155196 (2020)

## **52 Structure and properties of CoCrFeNiX multi-principal element alloys from ab initio calculations**

Koval NE, Juaristi JI, Muino RD, and Alducin M.  
Journal of Applied Physics 127, 145102 (2020)

## **53 Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems**

Tancogne-Dejean N, Oliveira MJT, Andrade X, Appel H, Borca CH, Le Breton G, Buchholz F, Castro A, Corni S, Correa AA, De Giovannini U, Delgado A, Bich FG, Flick J, Gil G, Gomez A, Helbig N, Hubener H, Jestadt R, Jornet-Somoza J, Larsen AH, Lebedeva IV, Luders M, Marques MAL, Ohlmann ST, Pipolo S, Rampp M, Rozzi CA, Strubbe DA, Sato SA, Schafer C, Theophilou I, Welden A, and Rubio A.  
Journal of Chemical Physics 152, 124119 (2020)

## **54 Siesta: Recent developments and applications**

Garcia A, Papior N, Akhtar A, Artacho E, Blum V, Bosoni E, Brandimarte P, Brandbyge M, Cerda JI, Corsetti F, Cuadrado R, Dikan V, Ferrer J, Gale J, Garcia-Fernandez P, Garcia-Suarez VM, Garcia S, Huhs G, Illera S, Korytar R, Koval P, Lebedeva I, Lin L, Lopez-Tarifa P, Mayo SG, Mohr S, Ordejon P, Postnikov A, Pouillon Y, Pruneda M, Robles R, Sanchez-Portal D, Soler JM, Ullah R, Yu VWZ, and Junquera J.  
Journal of Chemical Physics 152, 204108 (2020)

## **55 On the microscopic origins of relaxation processes in aqueous peptide solutions undergoing a glass transition**

Weigler M, Combarro-Palacios I, Cerveny S, and Vogel M.  
Journal of Chemical Physics 152, 234503 (2020)

## **56 The CECAM electronic structure library and the modular software development paradigm**

Oliveira MJT, Papior N, Pouillon Y, Blum V, Artacho E, Caliste D, Corsetti F, de Gironcoli S, Elena AM, Garcia A, Garcia-Suarez VM, Genovese L, Huhn WP, Huhs G, Kokott S, Kucukbenli E, Larsen AH, Lazzaro A, Lebedeva IV, Li YZ, Lopez-Duran D, Lopez-Tarifa P, Luders M, Marques MAL, Minar J, Mohr S, Mostofi AA, O'Cais A, Payne MC, Ruh T, Smith DGA, Soler JM, Strubbe DA, Tancogne-Dejean N, Tildesley D, Torrent M, and Yu VWZ.  
Journal of Chemical Physics 153, 24117 (2020)

## **57 Effect of many modes on self-polarization and photochemical suppression in cavities**

Hoffmann NM, Lacombe L, Rubio A, and Maitra NT.  
Journal of Chemical Physics 153, 104103 (2020)

## **58 Time-dependent magnons from first principles**

Tancogne-Dejean N, Eich FG, and Rubio A.  
Journal of Chemical Theory and Computation 16, 1007 (2020)

## **59 Deformability and solvent penetration in soft nanoparticles at liquid-liquid interfaces**

Arismendi-Arrieta DJ, and Moreno AJ.  
Journal of Colloid and Interface Science 570, 212 (2020)

# PUBLICATIONS

---

**60 Oxygen doping and polaron magnetic coupling in Alq<sub>3</sub> films**

Droghetti A.

Journal of Magnetism and Magnetic Materials 502, 166578 (2020)

**61 4-Miktoarm star architecture induces PVDF beta-phase formation in (PVDF)<sub>2</sub>-b-(PEO)<sub>2</sub> miktoarm star copolymers**

Maria N, Maiz J, Rodionov V, Hadjichristidis N, and Muller AJ.

Journal of Materials Chemistry C 8, 13786 (2020)

**62 Harvesting multiple optical energies using ZnPc/CdS-QDs hybrid organic/inorganic semiconductors**

El-Sayed A, Mahdy IA, Ibraheem F, Mahmoud EA, and Ortega JE.

Journal of Materials Science-Materials in Electronics 31, 12735 (2020)

**63 Insights into the non-exponential behavior of the dielectric Debye-like relaxation in monoalcohols**

Arrese-Igor S, Alegria A, Arbe A, and Colmenero J.

Journal of Molecular Liquids 312, 113441 (2020)

**64 Signature of hydrogen bonding association in the dielectric signal of polyalcohols**

Arrese-Igor S, Alegria A, and Colmenero J.

Journal of Molecular Liquids 318, 114215 (2020)

**65 Efficient ab initio multiplet calculations for magnetic adatoms on MgO**

Wolf C, Delgado F, Reina J, and Lorente N.

Journal of Physical Chemistry A 124, 2318 (2020)

**66 Magnetism and distortions in two-dimensional transition-metal dioxides: On the quest for intrinsic magnetic semiconductor layers**

Aguilera-Granja F, and Ayuela A.

Journal of Physical Chemistry C 124, 2634 (2020)

**67 Anisotropic PC<sub>6</sub>N monolayer with wide band gap and ultrahigh carrier mobility**

Wang C, Yu T, Bergara A, Du X, Li F, and Yang GC.

Journal of Physical Chemistry C 124, 4330 (2020)

**68 Directionality in Van der Waals Interactions: The Case of 4-Acetylbiphenyl adsorbed on Au(111)**

Zobac V, Robles R, and Lorente N.

Journal of Physical Chemistry C 124, 4545 (2020)

**69 Influence of the chemical structure on molecular light emission in strongly localized plasmonic fields**

Zhang Y, Dong ZC, and Aizpurua J.

Journal of Physical Chemistry C 124, 4674 (2020)

**70 CO chemisorption on vicinal Rh(111) surfaces studied with a curved crystal**

Garcia-Martinez F, Schiller F, Blomberg S, Shipilin M, Merte LR, Gustafson J, Lundgren E, and Ortega JE.

Journal of physical Chemistry C 124, 9305 (2020)

# PUBLICATIONS

---

## **71 Synthesis of graphene nanoribbons on a kinked Au surface: Revealing the frontier valence band at the brillouin zone center**

El-Sayed A, Piquero-Zulaica I, Abd El-Fattah ZM, Kormos L, Ali K, Weber A, Brede J, de Oteyza DG, Lobo-Checa J, Ortega JE, and Corso M.

Journal of Physical Chemistry C 124, 15474 (2020)

## **72 Increase of polymerization yield on Titania by surface reduction**

Abadia M, Vasseur G, Kolmer M, Zajac L, Verdini A, Ortega JE, Floreano L, Rogero C, and Brede J.

Journal of Physical Chemistry C 124, 16918 (2020)

## **73 Surface phase nucleation of lead monoatomic layers on Si(111) induced by Manganese Phthalocyanine molecules**

Longo D, Bocquet ML, Lorente N, Cruguel H, Debontridder F, Royer S, David P, Palacio-Morales A, Cren T, Witkowski N, and Brun C.

Journal of Physical Chemistry C 124, 19829 (2020)

## **74 Energy-based plasmonic index to characterize optical resonances in nanostructures**

Muller MM, Kosik M, Pelc M, Bryant GW, Ayuela A, Rockstuhl C, and Slowik K.

Journal of Physical Chemistry C 124, 24331 (2020)

## **75 Deep-glassy ice VI revealed with a combination of neutron spectroscopy and diffraction**

Rosu-Finsen A, Amon A, Armstrong J, Fernandez-Alonso F, and Salzmann CG.

Journal of Physical Chemistry Letters 11, 1106 (2020)

## **76 On-surface synthesis of a five-membered carbon ring from a terminal alkynyl bromide: A [4+1] annulation**

Wang T, Pan Y, Zhang WZ, Lawrence J, Mohammed MSG, Huang JM, Feng L, Berdonces-Layunta A, Han D, Xu Q, Wu XJ, Tait SL, de Oteyza DG, and Zhu JF.

Journal of Physical Chemistry Letters 11, 5902 (2020)

## **77 Transmitting stepwise rotation among three molecule-gear on the Au(111) surface**

Yeung KHA, Kuhne T, Eisenhut F, Kleinwachter M, Gisbert Y, Robles R, Lorente N, Cuniberti G, Joachim C, Rapenne G, Kammerer C, and Moresco F.

Journal of Physical Chemistry Letters 11, 6892 (2020)

## **78 Key role of the surface band structure in spin-dependent interfacial electron transfer: Ar/Fe(110) and Ar/Co(0001)**

Muller M, Echenique PM, and Sanchez-Portal D.

Journal of Physical Chemistry Letters 11, 7141 (2020)

## **79 Chemistry in quantum cavities: Exact results, the impact of thermal velocities, and modified dissociation**

Sidler D, Ruggenthaler M, Appel H, and Rubio A.

Journal of Physical Chemistry Letters 11, 7525 (2020)

## **80 Synergy of excitation enhancement and the purcell effect for Strong photoluminescence enhancement in a thin-film hybrid structure based on quantum dots and plasmon nanoparticles**

Krivenkov V, Samokhvalov P, Nabiev I, and Rakovich YP.

Journal of Physical Chemistry Letters 11, 8018 (2020)



## **81 On-surface synthesis of chlorinated narrow graphene nanoribbon organometallic hybrids**

Zuzak R, Brandimarte P, Olszowski P, Izydorchyk I, Markoulides M, Such B, Kolmer M, Szymonski M, Garcia-Lekue A, Sanchez-Portal D, Gourdon A, and Godlewski S.  
Journal of Physical Chemistry Letters 11, 10290 (2020)

## **82 Spectral and optical properties of $\text{Ag}_3\text{Au}(\text{Se}_2, \text{Te}_2)$ and dark matter detection**

Sanchez-Martinez MA, Robredo I, Bidaurrezaga A, Bergara A, de Juan F, Grushin AG, and Vergniory MG.  
Journal of Physics- Materials 3, 14001 (2020)

## **83 Wannier90 as a community code: new features and applications**

Pizzi G, Vitale V, Arita R, Blugel S, Freimuth F, Geranton G, Gibertini M, Gresch D, Johnson C, Koretsune T, Ibanez-Azpiroz J, Lee H, Lihm JM, Marchand D, Marrazzo A, Mokrousov Y, Mustafa JI, Nohara Y, Nomura Y, Paulatto L, Ponce S, Ponweiser T, Qiao JF, Thole F, Tsirkin SS, Wierzbowska M, Marzari N, Vanderbilt D, Souza I, Mostofi AA, and Yates JR.  
Journal of Physics-Condensed Matter 32, 165902 (2020)

## **84 Dominant contributions to the apparent activation energy in two-dimensional submonolayer growth: comparison between Cu/Ni(111) and Ni/Cu(111)**

Alberdi-Rodriguez J, Acharya SR, Rahman TS, Arnau A, and Gosálvez MA.  
Journal of Physics-Condensed Matter 32, 445002 (2020)

## **85 Crystal analyzers for indirect-geometry broadband neutron spectrometers: Adding reality to idealized design**

Zanetti M, Masi F, Rudic S, Armstrong J, Parker SF, Fernandez-Alonso F, and Gorini G.  
Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques 14, 242 (2020)

## **86 Covalent C-N bond formation through a surface catalyzed thermal Cyclodehydrogenation**

Piskun I, Blackwell R, Jornet-Somoza J, Zhao FZ, Rubio A, Louie SG, and Fischer FR.  
Journal of the American Chemical Society 142, 3696 (2020)

## **87 The subchalcogenides $\text{Ir}_2\text{In}_3\text{Q}$ (Q = S, Se, Te): Dirac semimetal candidates with Re-entrant structural modulation**

Khoury JF, Rettie AJE, Robredo I, Krogstad MJ, Malliakas CD, Bergara A, Vergniory MG, Osborn R, Rosenkranz S, Chung DY, and Kanatzidis MG.  
Journal of the American Chemical Society 142, 6312 (2020)

## **88 Inducing open-shell character in porphyrins through surface-assisted phenalenyl pi-extension**

Sun Q, Mateo LM, Robles R, Ruffieux P, Lorente N, Bottari G, Torres T, and Fasel R.  
Journal of the American Chemical Society 142, 18109 (2020)

## **89 Characterization of comb shaped MAA-co-PEGMA copolymers synthesized by free-radical polymerization**

Emaldi I, Agirre A, Etxeberria A, Erkizia E, Dolado JS, and Leiza JR.  
Macromolecular Reaction Engineering 14, 2000015 (2020)

## **90 Poly(ethylene oxide) melt intercalation in graphite oxide: Sensitivity to topology, cyclic versus linear chains**

Barroso-Bujans F, Allgaier J, and Alegria A.  
Macromolecules 53, 406 (2020)

**91 High lithium conductivity of miscible PEO/methacrylic sulfonamide anionic polyelectrolyte polymer blends**

Olmedo-Martínez JL, Porcarelli L, Alegría A, Mecerreyes D, and Müller AJ.  
Macromolecules 53, 4442 (2020)

**92 Free volume in a PVME polymer-water solution**

Capponi S, Alvarez F, and Racko D.  
Macromolecules 53, 4770 (2020)

**93 How does microstructural design affect the dynamics and rheology of segmented polyurethanes?**

Heydarnezhad HR, Mohammadi N, Arbe A, and Alegría A.  
Macromolecules 53, 5381 (2020)

**94 Tube dilation in isofrictional polymer blends based on polyisoprene with different topologies: Combination of dielectric and rheological spectroscopy, pulsed-field-gradient NMR, and Neutron Spin Echo (NSE) techniques**

De Molina PM, Alegría A, Allgaier J, Kruteva M, Hoffmann I, Prevost S, Monkenbusch M, Richter D, Arbe A, and Colmenero J.  
Macromolecules 53, 5919 (2020)

**95 Effect of nanoconfinement on the isodimorphic crystallization of poly(butylene succinate-ran-caprolactone) random copolymers**

Safari M, Boigues LL, Shi GY, Maiz J, Liu GM, Wang DJ, Mijangos C, and Muller AJ.  
Macromolecules 53, 6486 (2020)

**96 Concentration fluctuations and nanosegregation in a simplified industrial blend with large dynamic asymmetry**

Gambino T, Shafqat N, Alegría A, Malicki N, Dronet S, Radulescu A, Nemkovski K, Arbe A, and Colmenero J.  
Macromolecules 53, 7150 (2020)

**97 Structure and dynamics of irreversible single-chain nanoparticles in dilute solution. A neutron scattering investigation**

Gonzalez-Burgos M, Asenjo-Sanz I, Pomposo JA, Radulescu A, Ivanova O, Pasini S, Arbe A, and Colmenero J.  
Macromolecules 53, 8068 (2020)

**98 Partition of coating agents between nanoparticle interfaces and the polymer in nanocomposites**

Musino D, Oberdisse J, Sztucki M, Alegría A, and Genix AC.  
Macromolecules 53, 8083 (2020)

**99 Physical aging and glass transition of the rigid amorphous fraction in poly(L-lactic acid)**

Monnier X, Cavallo D, Righetti MC, Di Lorenzo ML, Marina S, Martin J, and Cangialosi D.  
Macromolecules 53, 8741 (2020)

**100 Synthesis of macrocyclic poly(glycidyl phenyl ether) with an inverted-dipole microstructure via ring closure of two-arm linear precursors obtained by initiation with t-BuP4/Water**

Ochs J, Alegría A, Roman EGD, Grayson SM, and Barroso-Bujans F.  
Macromolecules 53, 10005 (2020)

# PUBLICATIONS

---

## **101 Evidence of nanostructure development from the molecular dynamics of poly(pentamethylene 2,5-furanoate)**

Martinez-Tong DE, Soccio M, Robles-Hernandez B, Guidotti G, Gazzano M, Lotti N, and Alegria A.  
Macromolecules 53, 10526 (2020)

## **102 Elucidation of conduction mechanism in graphene nanoplatelets (GNPs)/cement composite using dielectric spectroscopy**

Goracci G, and Dolado JS.  
Materials 13, 275 (2020)

## **103 THz fingerprints of cement-based materials**

Dolado JS, Goracci G, Duque E, Martauz P, Zuo YB, and Ye G.  
Materials 13, 4194 (2020)

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

Verde-Sesto E, Arbe A, Moreno AJ, Cangialosi D, Alegria A, Colmenero J, and Pomposo JA.  
Materials Horizons 7, 2292 (2020)

## **105 KIMERA: A kinetic montecarlo code for mineral dissolution**

Martin P, Gaitero JJ, Dolado JS, and Manzano H.  
Minerals 10, 825 (2020)

## **106 On-surface atom-by-atom-assembled aluminum binuclear tetrabenzophenazine organometallic magnetic complex**

Soe WH, Manzano C, Robles R, Lorente N, and Joachim C.  
Nano Letters 20, 384 (2020)

## **107 Anharmonicity and doping melt the charge density wave in single-layer $\text{TiSe}_2$**

Zhou JQS, Monacelli L, Bianco R, Errea I, Mauri F, and Calandra M.  
Nano Letters 20, 4809 (2020)

## **108 Visualization of multifractal superconductivity in a two-dimensional transition metal dichalcogenide in the weak-disorder regime**

Rubio-Verdu C, Garcia-Garcia AM, Ryu HJ, Choi DJ, Zaldivar J, Tang SJ, Fan B, Shen ZX, Mo SK, Pascual JI, and Ugeda MM.  
Nano Letters 20, 5111 (2020)

## **109 Room temperature terahertz electroabsorption modulation by excitons in monolayer transition metal dichalcogenides**

Shi JJ, Baldini E, Latini S, Sato SA, Zhang YQ, Pein BC, Shen PC, Kong J, Rubio A, Gedik N, and Nelson KA.  
Nano Letters 20, 5214 (2020)

## **110 Strong interfacial exchange field in a heavy metal/ferromagnetic insulator system determined by spin hall magnetoresistance**

Gomez-Perez JM, Zhang XP, Calavalle F, Ilyn M, Gonzalez-Orellana C, Gobbi M, Rogero C, Chuvilin A, Golovach VN, Hueso LE, Bergeret FS, and Casanova F.  
Nano Letters 20, 6815 (2020)

# PUBLICATIONS

---

## **111 The Kondo effect of a molecular tip as a magnetic sensor**

Garnier L, Verlhac B, Abufager P, Lorente N, Ormaza M, and Limot L.  
Nano Letters 20, 8193 (2020)

## **112 Charge-transfer plasmon polaritons at graphene/alpha-RuCl<sub>3</sub> interfaces**

Rizzo DJ, Jessen BS, Sun ZY, Ruta FL, Zhang J, Yan JQ, Xian LD, McLeod AS, Berkowitz ME, Watanabe K, Taniguchi T, Nagler SE, Mandrus DG, Rubio A, Fogler MM, Millis AJ, Hone JC, Dean CR, and Basov DN.  
Nano Letters 20, 8438 (2020)

## **113 Tunable photodetectors via in situ thermal conversion of TiS<sub>3</sub> to TiO<sub>2</sub>**

Ghasemi F, Frisenda R, Flores E, Papadopoulos N, Biele R, de Lara DP, van der Zant HSJ, Watanabe K, Taniguchi T, D'Agosta R, Ares JR, Sanchez C, Ferrer IJ, and Castellanos-Gomez A.  
Nanomaterials 10, 711 (2020)

## **114 Non-linear optical properties of Er<sup>3+</sup>-Yb<sup>3+</sup>-doped NaGdF<sub>4</sub> nanostructured glass-ceramics**

Velazquez JJ, Gorni G, Balda R, Fernandez J, Pascual L, Duran A, and Pascual MJ.  
Nanomaterials 10, 1425 (2020)

## **115 Quantum theory of surface-enhanced resonant Raman scattering (SERRS) of molecules in strongly coupled plasmon-exciton systems**

Neuman T, Aizpurua J, and Esteban R.  
Nanophotonics 9, 295 (2020)

## **116 Independent engineering of individual plasmon modes in plasmonic dimers with conductive and capacitive coupling**

Krapek V, Konecna A, Horak M, Ligmajer F, Stoger-Pollach M, Hrton M, Babock J, and Sikola T.  
Nanophotonics 9, 623 (2020)

## **117 Nanofocusing of acoustic graphene plasmon polaritons for enhancing mid-infrared molecular fingerprints**

Voronin KV, Aguirreche UA, Hillenbrand R, Volkov VS, Alonso-Gonzalez P, and Nildtin AY.  
Nanophotonics 9, 2089 (2020)

## **118 Strongly coupled exciton-plasmon nanohybrids reveal extraordinary resistance to harsh environmental stressors: temperature, pH and irradiation**

Hendel T, Krivenkov V, Sanchez-Iglesias A, Grzelczak M, and Rakovich YP.  
Nanoscale 12, 16875 (2020)

## **119 Influence of 4f filling on electronic and magnetic properties of rare earth-Au surface compounds**

Fernandez L, Blanco-Rey M, Castrillo-Bodero R, Ilyn M, Ali K, Turco E, Corso M, Ormaza M, Gargiani P, Valbuena MA, Mugarza A, Moras P, Sheverdyeva PM, Kundu AK, Jugovac M, Laubschat C, Ortega JE, and Schiller F.  
Nanoscale 12, 22258 (2020)

## **120 See how atoms dance**

Aizpurua J.  
National Science Review 7, 833 (2020)

## **121 Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride**

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

Nature 578, 66 (2020)

## **122 Fluorescent bicolour sensor for low-background neutrinoless double beta decay experiments**

Rivilla I, Aparicio B, Bueno JM, Casanova D, Tonnele C, Freixa Z, Herrero P, Rogero C, Miranda JI, Martinez-Ojeda RM, Monrabal F, Olave B, Schafer T, Artal P, Nygren D, Cossio FP, and Gomez-Cadenas JJ.

Nature 583, 48 (2020)

## **123 Flickering nanometre-scale disorder in a crystal lattice tracked by plasmonic flare light emission**

Carnegie C, Urbieta M, Chikkaraddy R, de Nijs B, Griffiths J, Deacon WM, Kamp M, Zabala N, Aizpurua J, and Baumberg JJ.

Nature Communications 11, 682 (2020)

## **124 One-dimensional flat bands in twisted bilayer germanium selenide**

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

Nature Communications 11, 1124 (2020)

## **125 Polycyclic aromatic chains on metals and insulating layers by repetitive [3+2] cycloadditions**

Riss A, Richter M, Paz AP, Wang XY, Raju R, He YQ, Ducke J, Corral E, Wuttke M, Seufert K, Garnica M, Rubio A, Barth JV, Narita A, Mullen K, Berger R, Feng XL, Palma CA, and Auwärter W.

Nature Communications 11, 1490 (2020)

## **126 Vibron-assisted spin excitation in a magnetically anisotropic molecule**

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

Nature Communications 11, 1619 (2020)

## **127 Direct observation of desorption of a melt of long polymer chains**

Monnier X, Napolitano S, and Cangialosi D.

Nature Communications 11, 4354 (2020)

## **128 Graphene transistors for real-time monitoring molecular self-assembly dynamics**

Gobbi M, Galanti A, Stoeckel MA, Zyska B, Bonacchi S, Hecht S, and Samori P.

Nature Communications 11, 4731 (2020)

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

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

Nature Communications 11, 4821 (2020)

# PUBLICATIONS

---

## **130 Correlated electronic phases in twisted bilayer transition metal dichalcogenides**

Wang L, Shih EM, Ghiotto A, Xian L, Rhodes DA, Tan C, Claassen M, Kennes DM, Bai YS, Kim B, Watanabe K, Taniguchi T, Zhu XY, Hone J, Rubio A, Pasupathy AN, and Dean CR.  
Nature Materials 19, 861 (2020)

## **131 Broad spectral tuning of ultra-low-loss polaritons in a Van der Waals crystal by intercalation**

Taboada-Gutierrez J, Alvarez-Perez G, Duan JH, Ma WL, Crowley K, Prieto I, Bylinkin A, Autore M, Volkova H, Kimura K, Berger MH, Li SJ, Bao QL, Gao XPA, Errea I, Nikitin AY, Hillenbrand R, Martin-Sanchez J, and Alonso-Gonzalez P.  
Nature Materials 19, 964 (2020)

## **132 Single-molecule tautomerization tracking through space- and time-resolved fluorescence spectroscopy**

Doppagne B, Neuman T, Soria-Martinez R, Lopez LEP, Bulou H, Romeo M, Berciaud S, Scheurer F, Aizpurua J, and Schull G.  
Nature Nanotechnology 15, 207 (2020)

## **133 Topological engineering for metallic polymers**

Corso M, and de Oteyza DG.  
Nature Nanotechnology 15, 421 (2020)

## **134 A Josephson phase battery**

Strambini E, Iorio A, Durante O, Citro R, Sanz-Fernandez C, Guarcello C, Tokatly IV, Braggio A, Rocci M, Ligato N, Zannier V, Sorba L, Bergeret FS, and Giazotto F.  
Nature Nanotechnology 15, 656 (2020)

## **135 Sub-nanometre resolution in single-molecule photoluminescence imaging**

Yang B, Chen G, Ghafoor A, Zhang YF, Zhang Y, Zhang Y, Luo Y, Yang JL, Sandoghdar V, Aizpurua J, Dong ZC, and Hou JG.  
Nature Photonics 14, 693(2020)

## **136 Sub-femtosecond electron transport in a nanoscale gap**

Ludwig M, Aguirregabiria G, Ritzkowski F, Rybka T, Marinica DC, Aizpurua J, Borisov AG, Leitenstorfer A, and Brida D.  
Nature Physics 16, 341 (2020)

## **137 Symmetry-protection of multiphoton states of light**

Lasa-Alonso J, Molezuelas-Ferreras M, Varga JJM, Garcia-Etxarri A, Giedke G, and Molina-Terriza G.  
New Journal of Physics 22, 123010 (2020)

## **138 High-harmonic generation from spin-polarised defects in solids**

Mrudul MS, Tancogne-Dejean N, Rubio A, and Dixit G.  
NPJ Computational Materials 6, 10 (2020)

## **139 Tunable 3D/2D magnetism in the $(\text{MnBi}_2\text{Te}_4)_x(\text{Bi}_2\text{Te}_3)_{1-x}$ topological insulators family**

Klimovskikh II, Otrokov MM, Estyunin D, Ereemeev SV, Filnov SO, Koroleva A, Shevchenko E, Voroshnin V, Rybkin AG, Rusinov IP, Blanco-Rey M, Hoffmann M, Aliev ZS, Babanly MB, Amiraslanov IR, Abdullayev NA, Zverev VN, Kimura A, Tereshchenko OE, Kokh KA, Petaccia L, Di Santo G, Ernst A, Echenique PM, Mamedov NT, Shikin AM, and Chulkov EV.  
NPJ Quantum Materials 5, 54 (2020)

## **140 Dynamical amplification of electric polarization through nonlinear phononics in 2D SnTe**

Shin DB, Sato SA, Hubener H, De Giovannini U, Park N, and Rubio A.

NPJ Quantum Materials 6, 182 (2020)

## **141 The instrument suite of the European Spallation Source**

Andersen KH, Argyriou DN, Jackson AJ, Houston J, Henry PF, Deen PP, Toft-Petersen R, Beran P, Strobl M, Arnold T, Wacklin-Knecht H, Tsapatsaris N, Oksanen E, Woracek R, Schweika W, Mannix D, Hiess A, Kennedy S, Kirstein O, Arskold SP, Taylor J, Hagen ME, Laszlo G, Kanaki K, Piscitelli F, Khaplanov A, Stefanescu I, Kittelmann T, Pfeiffer D, Hall-Wilton R, Lopez CI, Aprigliano G, Whitelegg L, Moreira FY, Olsson M, Bordallo HN, Martin-Rodriguez D, Schneider H, Sharp M, Hartl M, Nagy G, Ansell S, Pullen S, Vickery A, Fedrigo A, Mezei F, Arai M, Heenan RK, Halcrow W, Turner D, Raspino D, Orszulik A, Cooper J, Webb N, Galsworthy P, Nightingale J, Langridge S, Elmer J, Frielinghaus H, Hanslik R, Gussen A, Jaksch S, Engels R, Kozielowski T, Butterweck S, Feyngenson M, Harbott P, Poque A, Schwaab A, Lieutenant K, Violini N, Voigt J, Bruckel T, Koenen M, Kammerling H, Babcock E, Salhi Z, Wischniewski A, Heynen A, Desert S, Jestin J, Porcher F, Fabreges X, Fabreges G, Annighofer B, Klimko S, Dupont T, Robillard T, Goukassov A, Longeville S, Alba-Simionesco C, Bourges P, Le Bouffy JG, Lavie P, Rodrigues S, Calzada E, Lerche M, Schillinger B, Schmakat P, Schulz M, Seifert M, Lohstroh W, Petry W, Neuhaus J, Loaiza L, Tartaglione A, Glavic A, Schutz S, Stahn J, Lehmann E, Morgano M, Schefer J, Filges U, Klauser C, Niedermayer C, Fenske J, Nowak G, Rouijaa M, Siemers DJ, Kiehn R, Muller M, Carlsen H, Udby L, Lefmann K, Birk JO, Holm-Dahlin S, Bertelsen M, Hansen UB, Olsen MA, Christensen M, Iversen K, Christensen NB, Ronnow HM, Freeman PG, Hauback BC, Kolevator R, Llamas-Jansa I, Orecchini A, Sacchetti F, Petrillo C, Paciaroni A, Tozzi P, Zanatta M, Luna P, Herranz I, del Moral OG, Huerta M, Magan M, Mosconi M, Abad E, Aguilar J, Stepanyan S, Bakedano G, Vivanco R, Bustinduy I, Sordo F, Martinez JL, Lechner RE, Villacorta FJ, Saroun J, Lukas P, Marko M, Zanetti M, Bellissima S, del Rosso L, Masi F, Bovo C, Chowdhury M, De Bonis A, Di Fresco L, Scatigno C, Parker SF, Fernandez-Alonso F, Colognesi D, Senesi R, Andreani C, Gorini G, Scionti G, and Schreyer A.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment 957, 163402 (2020)

## **142 Swift charged particles in a degenerate electron gas: An estimation for the charge-sign effect in stopping**

Nagy I, and Aldazabal I.

Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms 474, 74 (2020)

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

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

Optical Materials Express 10, 2695 (2020)

## **144 Magnetic modulation of far- and near-field IR properties in rod-slit complementary spintronic metasurfaces**

Armelles G, Bergamini L, Cebollada A, Gonzalez MU, Alvaro R, Torn L, Zabala N, and Aizpurua J.

Optics Express 28, 32584 (2020)

## **145 Enhanced thermopower in covalent graphite-molecule contacts**

Droghetti A, and Rungger I.

Physical Chemistry Chemical Physics 22, 1466 (2020)

## **146 On the microscopic origin of the cryoprotective effect in lysine solutions**

Henao A, Ruiz GN, Steinke N, Cerveny S, Macovez R, Guardia E, Busch S, McLain SE, Lorenz CD, and Pardo LC.

Physical Chemistry Chemical Physics 22, 6919 (2020)

# PUBLICATIONS

---

## **147 Supramolecular chemistry based on 4-acetylbiphenyl on Au(111)**

Robles R, Zobac V, Yeung KHA, Moresco F, Joachim C, and Lorente N.  
Physical Chemistry Chemical Physics 22, 15208 (2020)

## **148 Steric clash in real space: biphenyl revisited**

Laplaza R, Boto RA, Contreras-Garcia J, and Montero-Campillo MM.  
Physical Chemistry Chemical Physics 22, 21251 (2020)

## **149 When classical trajectories get to quantum accuracy. II. The scattering of rotationally excited H<sub>2</sub> on Pd(111)**

Rodriguez-Fernandez A, Bonnet L, Crespos C, Larregaray P, and Muino RD.  
Physical Chemistry Chemical Physics 22, 22805 (2020)

## **150 Achieving high hydrogen evolution reaction activity of a Mo<sub>2</sub>C monolayer**

Lou H, Yu T, Ma JN, Zhang ST, Bergara A, and Yang GC.  
Physical Chemistry Chemical Physics 22, 26189 (2020)

## **151 Exact exchange-correlation potential of effectively interacting Kohn-Sham systems**

Sato SA, and Rubio A.  
Physical Review A 101, 12510 (2020)

## **152 Two-channel approach to the average retarding force of metals for slow singly ionized projectiles**

Nagy I, and Aldazabal I.  
Physical Review A 102, 32814 (2020)

## **153 Berezinskii-Kosterlitz-Thouless transition in two-dimensional dipolar stripes**

Bombin R, Mazzanti F, and Boronat J.  
Physical Review A 102, 47302 (2020)

## **154 Cryogenic memory element based on an anomalous Josephson junction**

Guarcello C, and Bergeret FS.  
Physical Review Applied 13, 34012 (2020)

## **155 Plasmonic antennas with electric, magnetic, and electromagnetic hot spots based on Babinet's principle**

Hrton M, Konecna A, Horak M, Sikola T, and Krapek V.  
Physical Review Applied 13, 54045 (2020)

## **156 Prediction of superconductivity in pressure-induced new silicon boride phases**

Liang XW, Bergara A, Xie Y, Wang LY, Sun RX, Gao YF, Zhou XF, Xu B, He JL, Yu DL, Gao GY, and Tian YJ.  
Physical Review B 101, 14112 (2020)

## **157 Spin dependent transmission of nickelocene-Cu contacts probed with shot noise**

Mohr M, Gruber M, Weismann A, Jacob D, Abufager P, Lorente N, and Berndt R.  
Physical Review B 101, 75414 (2020)

## **158 Axion coupling in the hybrid Wannier representation**

Varnava N, Souza I, and Vanderbilt D.  
Physical Review B 101, 155130 (2020)



# PUBLICATIONS

---

## **159 Superconducting boron allotropes**

Zhang ST, Du X, Lin JY, Bergara A, Chen X, Liu XB, Zhang XH, Yang GC  
Physical Review B 101, 174507 (2020)

## **160 Phase-controllable nonlocal spin polarization in proximitized nanowires**

Zhang XP, Golovach VN, Giazotto F, and Bergeret FS.  
Physical Review B 101, 180502 (2020)

## **161 Interplay between superconductivity and spin-dependent fields in nanowire-based systems**

Baumard J, Cayssol J, Buzdin A, and Bergeret FS.  
Physical Review B 101, 184512 (2020)

## **162 Nanomechanics of a hydrogen molecule suspended between two equally charged tips**

Schattke W, Frederiksen T, Van Hove MA, and Muino RD.  
Physical Review B 101, 195436 (2020)

## **163 Spin-orbit splitting of quantum well states in n-monolayer Ir/Au(111) heterostructures**

Silkin IV, Koroteev YM, Silkin VM, and Chulkov EV.  
Physical Review B 101, 235409 (2020)

## **164 Active control of ultrafast electron dynamics in plasmonic gaps using an applied bias**

Ludwig M, Kazansky AK, Aguirregabiria G, Marinica DC, Falk M, Leitenstorfer A, Brida D, Aizpurua J, and Borisov AG.  
Physical Review B 101, 241412 (2020)

## **165 Constraint-based wave vector and frequency dependent exchange-correlation kernel of the uniform electron gas**

Ruzsinszky A, Nepal NK, Pitarke JM, and Perdew JP.  
Physical Review B 101, 245135 (2020)

## **166 Spin structure of spin-orbit split surface states in a magnetic material revealed by spin-integrated photoemission**

Usachov DY, Guttler M, Schulz S, Poelchen G, Seiro S, Kliemt K, Kummer K, Krellner C, Laubschat C, Chulkov EV, and Vyalikh DV.  
Physical Review B 101, 245140 (2020)

## **167 Collective excitations and universal broadening of cyclotron absorption in Dirac semimetals in a quantizing magnetic field**

Yasnov DI, Protogenov AP, Echenique PM, and Chulkov EV.  
Physical Review B 101, 245206 (2020)

## **168 Gapless hinge states from adiabatic pumping of axion coupling**

Olsen T, Rauch T, Vanderbilt D, and Souza I.  
Physical Review B 102, 35166 (2020)

## **169 Crossed graphene nanoribbons as beam splitters and mirrors for electron quantum optics**

Sanz S, Brandimarte P, Giedke G, Sanchez-Portal D, and Frederiksen T.  
Physical Review B 102, 35436 (2020)

## **170 Theory of the magnetic response in finite two-dimensional superconductors**

Bergeret FS, and Tokatly IV.

Physical Review B 102, 60506 (2020)

## **171 Electronic band structure of three-dimensional topological insulators with different stoichiometry composition**

Grimaldi I, Pacile D, Ereemeev SV, De Luca O, Policicchio A, Moras P, Sheverdyayeva PM, Kundu AK, Aliev ZS, Rudolf P, Agostino RG, Chukov EV, and Papagno M.

Physical Review B 102, 85118 (2020)

## **172 Probe-dependent Dirac-point gap in the gadolinium-doped thallium-based topological insulator**

**TlBi<sub>0.9</sub>Gd<sub>0.1</sub>Se<sub>2</sub>**

Filnov SO, Klimovskikh II, Estyunin DA, Fedorov AV, Voroshnin VY, Koroleva AV, Rybkin AG, Shevchenko EV, Aliev ZS, Babanly MB, Amiraslanov IR, Mamedov NT, Schwier EF, Miyamoto K, Okuda T, Kumar S, Kimura A, Misheneva VM, Shikin AM, and Chulkov EV.

Physical Review B 102, 85149 (2020)

## **173 Probing and steering bulk and surface phonon polaritons in uniaxial materials using fast electrons: Hexagonal boron nitride**

Maciel-Escudero C, Konecna A, Hillenbrand R, and Aizpurua J.

Physical Review B 102, 115431 (2020)

## **174 Parameter-free hybridlike functional based on an extended Hubbard model: DFT plus U plus V**

Tancogne-Dejean N, and Rubio A.

Physical Review B 102, 155117 (2020)

## **175 Electronic friction coefficients from the atom-in-jellium model for Z=1-92**

Gerrits N, Juaristi JI, and Meyer J.

Physical Review B 102, 155130 (2020)

## **176 Dual boson diagrammatic Monte Carlo approach applied to the extended Hubbard model**

Vandelli M, Harkov V, Stepanov EA, Gukelberger J, Kozik E, Rubio A, and Lichtenstein AI.

Physical Review B 102, 195109 (2020)

## **177 Topological phase transitions induced by disorder in magnetically doped (Bi, Sb)<sub>2</sub>Te<sub>3</sub> thin films**

Okugawa T, Tang PZ, Rubio A, and Kennes DM.

Physical Review B 102, 201405 (2020)

## **178 Photoelectron diffraction for probing valency and magnetism of 4 f-based materials: A view on valence-fluctuating EuR<sub>2</sub>Si<sub>2</sub>**

Usachov DY, Tarasov AV, Schulz S, Bokai KA, Tupitsyn II, Poelchen G, Seiro S, Caroca-Canales N, Kliemt K, Mende M, Kummer K, Krellner C, Muntwiler M, Li H, Laubschat C, Geibel C, Chulkov EV, Fujimori SI, and Vyalikh DV.

Physical Review B 102, 205102 (2020)

## **179 Unified description of spin transport, weak antilocalization, and triplet superconductivity in systems with spin-orbit coupling**

Ilic S, Tokatly IV, and Bergeret FS.

Physical Review B 102, 235430 (2020)

# PUBLICATIONS

---

## **180 Nature of symmetry breaking at the excitonic insulator transition: Ta<sub>2</sub>NiSe<sub>5</sub>**

Mazza G, Rosner M, Windgatter L, Latini S, Hubener H, Millis AJ, Rubio A, and Georges A.  
Physical Review Letters 124, 197601 (2020)

## **181 Cubic Rashba effect in the surface spin structure of rare-earth ternary materials**

Usachov DY, Nechaev IA, Poelchen G, Guttler M, ICrasovskii EE, Schulz S, Generalov A, Kliemt K, Kraiker A, Krellner C, Kummer K, Danzenbacher S, Laubschat C, Weber AP, Sanchez-Barriga J, Chulkov EV, Santander-Syro AF, Imai T, Miyamoto K, Okuda T, and Vyalikh DV.  
Physical Review Letters 124, 237202 (2020)

## **182 Kerker conditions upon lossless, absorption, and optical gain regimes**

Olmos-Trigo J, Sanz-Fernandez C, Abujetas DR, Lasa-Alonso J, de Sousa N, Garcia-Etxarri A, Sanchez-Gil JA, Molina-Terriza G, and Saenz JJ.  
Physical Review Letters 125, 73205 (2020)

## **183 Long-range propagation and interference of d-wave superconducting pairs in graphene**

Perconte D, Seurre K, Humbert V, Ulysse C, Sander A, Trastoy J, Zatko V, Godel F, Hofmann S, Bercioux D, Dlubak B, Seneor P, Villegas JE, Kidambi PR, Zhang XP, and Bergeret FS.  
Physical Review Letters 125, 87002 (2020)

## **184 Weak dimensionality dependence and dominant role of ionic fluctuations in the charge-density-wave transition of NbSe<sub>2</sub>**

Bianco R, Monacelli L, Calandra M, Mauri F, and Errea I.  
Physical Review Letters 125, 106101 (2020)

## **185 Giant exciton mott density in anatase TiO<sub>2</sub>**

Baldini E, Palmieri T, Dominguez A, Rubio A, and Chergui M.  
Physical Review Letters 125, 116403 (2020)

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

Friedrich N, Brandimarte P, Li JC, Saito S, Yamaguchi S, Pozo I, Pena D, Frederiksen T, Garcia-Lekue A, Sanchez-Portal D, and Pascual JI.  
Physical Review Letters 125, 146801 (2020)

## **187 Insight into the electronic structure of semiconducting epsilon-GaSe and epsilon-InSe**

Eremeev SV, Papagno M, Grimaldi I, De Luca O, Ferrari L, Kundu AK, Sheverdyayeva PM, Moras P, Avvisati G, Crepaldi A, Berger H, Vobornik I, Betti MG, Grioni M, Carbone C, Chulkov EV, and Pacile D.  
Physical Review Materials 4, 84603 (2020)

## **188 Living on the edge: Topology, electrostatics, and disorder**

van den Berg TL, Calvo MR, and Bercioux D.  
Physical Review Research 2, 13171 (2020)

## **189 Optimal backward light scattering by dipolar particles**

Olmos-Trigo J, Abujetas DR, Sanz-Fernandez C, Sanchez-Gil JA, and Saenz JJ.  
Physical review Research 2, 13225 (2020)

# PUBLICATIONS

---

## **190 Directional shift current in mirror-symmetric BC<sub>2</sub>N**

Ibanez-Azpiroz J, Souza I, and de Juan F.  
Physical Review Research 2, 13263 (2020)

## **191 Coherent structural relaxation of water from meso- to intermolecular scales measured using neutron spectroscopy with polarization analysis**

Arbe A, Nilsen GJ, Stewart JR, Alvarez F, Sakai VG, and Colmenero J.  
Physical Review Research 2, 22015 (2020)

## **192 rf-SQUID measurements of anomalous Josephson effect**

Guarcello C, Citro R, Durante O, Bergeret FS, Iorio A, Sanz-Fernandez C, Strambini E, Giazotto F, and Braggio A.  
Physical Review Research 2, 23165 (2020)

## **193 Unveiling dipolar spectral regimes of large dielectric Mie spheres from helicity conservation**

Olmos-Trigo J, Abujetas DR, Sanz-Fernandez C, Zambrana-Puyalto X, de Sousa N, Sanchez-Gil JA, and Saenz JJ.  
Physical Review Research 2, 43021 (2020)

## **194 Zero-point magnetic exchange interactions**

Bouaziz J, Ibanez-Azpiroz J, Guimaraes FSM, and Lounis S.  
Physical Review Research 2, 43357 (2020)

## **195 How circular dichroism in time- and angle-resolved photoemission can be used to spectroscopically detect transient topological states in graphene**

Schuler M, De Giovannini U, Hubener H, Rubio A, Sentef MA, Devereaux TP, and Werner P.  
Physical Review X 10, 41013 (2020)

## **196 Coupled cluster theory for molecular polaritons: Changing ground and excited states**

Haugland TS, Ronca E, Kjonstad EF, Rubio A, and Koch H.  
Physical Review X 10, 41043 (2020)

## **197 Modeling the high frequency mechanical relaxation of simplified industrial polymer mixtures using dielectric relaxation results**

Gambino T, Alegria A, Arbe A, Colmenero J, Malicki N, and Dronet S.  
Polymer 187, 122051 (2020)

## **198 From chemical structure to quantitative polymer properties prediction through convolutional neural networks**

Miccio LA, and Schwartz GA.  
Polymer 193, 122341 (2020)

## **199 Wrinkling poly(trimethylene 2,5-furanoate) free-standing films: Nanostructure formation and physical properties**

Soccio M, Lotti N, Munari A, Rebollar E, and Martinez-Tong DE.  
Polymer 202, 122666 (2020)

# PUBLICATIONS

---

## **200 Increasing the temperature range of dipolar glass polymers through copolymerization: A first approach to dipolar glass copolymers**

Bonardd S, Alegria A, Saldias C, Leiva A, and Kortaberria G.  
Polymer 203, 122765 (2020)

## **201 Localizing and quantifying the intra-monomer contributions to the glass transition temperature using artificial neural networks**

Miccio LA, and Schwartz GA.  
Polymer 203, 122786 (2020)

## **202 Poly(alkylene 2,5-furanoate)s thin films: Morphology, crystallinity and nanomechanical properties**

Robles-Hernandez B, Soccio M, Castrillo I, Guidotti G, Lotti N, Alegria A, and Martinez-Tong DE.  
Polymer 204, 122825 (2020)

## **203 SSAfractionation of thermoplastic polyurethanes**

Fernandez-d'Arlas B Maiz J, Perez-Camargo RA, Baumann RP, Poselt E, Dabbous R, and Stribeck A.  
Polymer Crystallization, e10148 (2020) (Early Access)

## **204 Coarsening kinetics of complex macromolecular architectures in bad solvent**

Paciolla M, Arismendi-Arrieta DJ, and Moreno AJ.  
Polymers 12, 531 (2020)

## **205 Dynamics of confined short-chain alkanol in MCM-41 by dielectric spectroscopy: Effects of matrix and system treatments and filling factor**

Bartos J, Arrese-Igor S, Svajdlenkova H, Kleinova A, and Alegria A.  
Polymers 12, 610 (2020)

## **206 Broadband dielectric spectroscopy study of biobased poly(alkylene 2,5-furanoate)s' molecular dynamics**

Soccio M, Martinez-Tong DE, Guidotti G, Robles-Hernandez B, Munari A, Lotti N, and Alegria A.  
Polymers 12, 1355 (2020)

## **207 Insight into the structure and dynamics of polymers by neutron scattering combined with atomistic molecular dynamics simulations**

Arbe A, Alvarez F, and Colmenero J.  
Polymers 12, 3067 (2020)

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

Maiz J, Verde-Sesto E, Asenjo-Sanz I, Fouquet P, Porcar L, Pomposo JA, de Molina PM, Arbe A, and Colmenero J.  
Polymers 13, 50 (2020)

## **209 Metallic bands in chevron-type polyacenes**

Kher-Elden MA, Piquero-Zulaica I, Abd El-Aziz KM, Ortega JE, and Abd El-Fattah ZM.  
RSC Advances 10, 33844 (2020)

# PUBLICATIONS

---

## **210 Weyl fermions, Fermi arcs, and minority-spin carriers in ferromagnetic CoS<sub>2</sub>**

Schroter NBM, Robredo I, Klemenz S, Kirby RJ, Krieger JA, Pei D, Yu TL, Stolz S, Schmitt T, Dudin P, Kim TK, Cacho C, Schnyder A, Bergara A, Strocov VN, de Juan F, Vergniory MG, and Schoop LM.  
Science Advances 6, 51 (2020)

## **211 Vitrification decoupling from alpha-relaxation in a metallic glass**

Monnier X, Cangialosi D, Ruta B, Busch R, and Gallino I.  
Science Advances 6, eaay1454 (2020)

## **212 Novel superhard boron-rich nitrides under pressure**

Wang LY, Sun RX, Liu WH, Yuan ZK, Bergara A, Liang XW, Chen S, Zhou XF, Xu B, He JL, Yu DL, Gao GY, and Tian YJ.  
Science China-Materials 63, 2358 (2020)

## **213 Nature of the Dirac gap modulation and surface magnetic interaction in axion antiferromagnetic topological insulator MnBi<sub>2</sub>Te<sub>4</sub>**

Shikin AM, Estyunin DA, Klimovskikh II, Filnov SO, Schwier EF, Kumar S, Miyamoto K, Okuda T, Kimura A, Kuroda K, Yaji K, Shin S, Takeda Y, Saitoh Y, Aliev ZS, Mamedov NT, Amiraslanov IR, Babanly MB, Otrokov MM, Ereemeev SV, and Chulkov EV.  
Scientific Reports 10, 13226 (2020)

## **214 Effect of environmental humidity on the ionic transport of poly(ethylene oxide) thin films, investigated by local dielectric spectroscopy**

Markus P, Martinez-Tong DE, Papastavrou G, and Alegria A.  
Soft Matter 16, 3203 (2020)

## **215 Distinct dynamics of structural relaxation in the amorphous phase of poly(L-lactic acid) revealed by quiescent crystallization**

Monnier X, Delpouve N, and Saiter-Fourcin A.  
Soft Matter 16, 3224 (2020)

## **216 Water dynamics and self-assembly of single-chain nanoparticles in concentrated solutions**

Robles-Hernandez B, Gonzalez E, Pomposo JA, Colmenero J, and Alegria A.  
Soft Matter 16, 9738 (2020)

## **217 NCIPLOT and the analysis of noncovalent interactions using the reduced density gradient**

Laplaza R, Peccati F, Boto RA, Quan CY, Carbone A, Piquemal JP, Maday Y, and Contreras-Garcia J.  
Wiley Interdisciplinary Reviews-Computational Molecular Science, e1497 (2020) (Early Access)

## Kimera (Software)

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

3905/2020

## Method for colorimetric detection of bacteria in food samples

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

20382599

## Sensible thermal energy storage media based on alkali activated concrete

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

20157518

## Superconducting electromagnetic wave sensor

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

WO 2019/058357 AI

## Superconducting logic element

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

WO 2019/038409 AI

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

Cervený S, and Swenson J.

Crystallization as Studied by Broadband dielectric spectroscopy- chapter 7, 167 (2020)

### Magnetic impurities on surfaces: Kondo and inelastic scattering

Choi DJ, and Lorente N.

Handbook of Materials Modeling: Applications: Current and Emerging Materials, 467 (2020)

### Enhancement of the quantum dot photoluminescence using transfer-printed porous silicon microcavities

Kryukova IS, Dovzhenko DS, Rakovich YP, and Nabiev IR.

Journal of Physics: Conference Series 1461, 012076 (2020)

### Glass transition and crystallization in colloidal polymer nanoparticles

Cangialosi D, and Nogales A.

Polymer Colloids: Formation, Characterization and Applications-Chapter 8, 263 (2020)

### Electronic states of vicinal surfaces

Ortega JE, Mugarza A, Schiller F, Lobo-Checa J, and Corso M.

Springer Handbook of Surface Science-Chapter 28, 351 (2020)

### Natural topological insulator heterostructures

Eremeev SV, Rusinov IP, and Chulkov EV.

Springer Handbook of Surface Science-Chapter 28, 449 (2020)

### Electron-phonon interaction on metallic surfaces, overlayers and thin films

Heid R, Sklyadneva IY, and Chulkov EV.

Springer Handbook of Surface Science-Chapter 28, 783 (2020)

### Nonadiabatic effects in gas-surface dynamics

Alducin M, Díez Muiño R, and Juaristi JI.

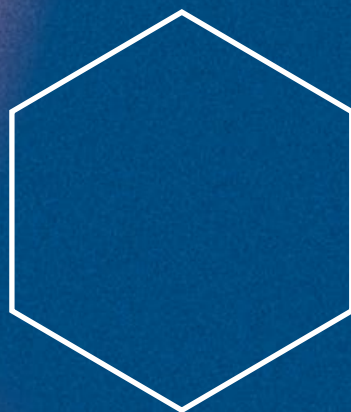
Springer Handbook of Surface Science-Chapter 28, 929 (2020)



# TRAINING ACTIVITIES

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

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



# TRAINING ACTIVITIES

## POST-DOCTORAL TRAINING

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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

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

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

## DEFENDED PHD THESES

- **Computational investigations of single-chain nanoparticles: Novel synthesis routes, complex flow behavior and reversible gel formation**  
Author: Maud Formanek  
Supervisor: Ángel Moreno Segurado  
Group: Polymers and Soft Matter  
19/01/2020
- **Quantum transport in nanowires with spin-orbit interaction effect of quasi-bound states**  
Author: Alba Pascual Gil  
Supervisors: F. Sebastián Bergeret Sbarbaro and Vitaly Golovach  
Group: Mesoscopic Physics  
03/03/2020
- **Molecular assembly and reactions on surfaces characterized by low-temperature scanning probe techniques**  
Author: Ana Barragán Durán  
Supervisor: Lucia Vitali  
Group: Spectroscopy at the Atomic Scale  
20/03/2020

- **Numerical simulations for the nonequilibrium control of quantum materials**  
 Author: Gabriel Topp  
 Supervisors: Michael Sentef and Ángel Rubio Secades  
 Group: Nano-Bio Spectroscopy  
 22/04/2020
- **Novel approaches in quantum chemistry: Self-consistent density-functional embedding and polaritonic coupled-cluster theory**  
 Author: Uliana Mordovina  
 Supervisors: Daniela Pfannkuche and Ángel Rubio Secades  
 Group: Nano-Bio Spectroscopy  
 27/04/2020
- **On the interface of quantum electrodynamics and electronic structure theory: Cavity QED**  
 Author: Christian Schaefer  
 Supervisors: Michael Ruggenthaler and Ángel Rubio Secades  
 Group: Nano-Bio Spectroscopy  
 13/05/2020
- **Mixed quantum-classical dynamics in cavity quantum electrodynamics**  
 Author: Norah Hoffmann  
 Supervisors: Neepa Maitra and Ángel Rubio Secades  
 Group: Nano-Bio Spectroscopy  
 02/06/2020
- **An efficient Ab-Initio non-equilibrium Green's function approach to carriers dynamics in many-body interacting systems**  
 Author: Fabio Covito  
 Supervisors: Daniela Pfannkuche and Ángel Rubio Secades  
 Group: Nano-Bio Spectroscopy  
 13/07/2020
- **Synthesis and characterization of cyclic polyethers with controlled orientation of the dipolar moment along the chain contour**  
 Author: Jordan Ochs  
 Supervisor: Fabienne Barroso Bujans  
 Group: Polymers and Soft Matter  
 09/09/2020
- **Anharmonic effects in thermoelectric and 2D materials**  
 Author: Unai Aseguinolaza Aguirreche  
 Supervisors: Ion Errea Lope and Aitor Bergara Jauregi  
 Group: Quantum Theory of Materials  
 18/09/2020

- **Spin-and valley-dependent transport in hybrid system and 2D Dirac materials**  
Author: Xianpeng Zhang  
Supervisors: F. Sebastián Bergeret Sbarbaro and Miguel Ángel Cazalilla Gutiérrez  
Group: Mesoscopic Physics  
12/12/2020
- **Many electrons and the photon field: The many-body structure of nonrelativistic quantum electrodynamics**  
Author: Florian Konrad Friedrich Buchholz  
Supervisors: Michael Ruggenthaler and Ángel Rubio Secades  
Group: Nano-Bio Spectroscopy  
24/11/2020

## SHORT STAYS IN FOREIGN UNIVERSITIES

A very important aspect of the PhD training program consists of supporting short stays in foreign universities and centers for PhD students. This year 6 PhD students have spent about 2-3 months in some of the best international centers on their topics. This training activity combines aspects of internationalization and excellence, and has been strongly supported within the last years by CFM. The following pre-doctoral researchers benefited from an internship abroad supported by CFM in 2020:

- **José Reina Gálvez**  
Universidad Nacional de San Martín, Buenos Aires (Argentina)  
29 February – 31 May
- **Masoud Mansouri**  
Boston University (USA)  
19 February - 8 May
- **Alvaro Nodar Villa**  
Macquarie University, Sidney (Australia)  
3 March - 10 May
- **Fernando García Martínez**  
Lund University (Sweden)  
4 October - 8 December
- **Mariarita Paciolla**  
University of Viena (Austria)  
9 September - 10 December
- **Cristina Mier González**  
IPCMS Strasbourg (France)  
21 September - 13 December

# MASTER EDUCATION PROGRAM

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## MASTER IN NANOSCIENCE

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

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

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

## SCHOLARSHIPS

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

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

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

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

## THESES OF THE NANOSCIENCE MASTER SUCCESSFULLY DEFENDED IN 2020

- **Infrared nanoimaging of ultraconfined surface phonon polaritons in MoS<sub>2</sub>-quartz heterostructures**  
Author: Petr Liska  
Supervisor: Rainer Hillenbrand (CIC nanoGUNE)
- **On the modelling of AFM-based nano-dielectric spectroscopy**  
Author: Jean Pierre Inchaustegui Revoredo  
Supervisors: Ángel Alegría Loinaz (CFM) and Daniel Martínez Tong (CFM)
- **Graphene nanoribbons with Carboxyl edge groups: On-surface synthesis and electronic characterization**  
Author: Lucie Pavlásková  
Supervisors: Aran García-Lekue (DIPC) and Martina Corso (CFM)
- **Anisotropy effect of nanostructure in the mechanical behaviour of pearlitic steel**  
Author: Aritz Dorronsoro Larbide  
Supervisor: Jon Alkorta Barragán (CEIT)
- **Anisotropic phonon polaritons in twisted biaxial Van der Waals crystal slabs**  
Author: Nathaniel Andrés Capote Robayna  
Supervisors: Alexey Nikitin (DIPC) and Pablo Alonso González (University of Oviedo)
- **DNA-Polymer hybrid nanostructures for stimuli-responsive systems**  
Author: Diego Ramírez Revilla  
Supervisor: Thomas Schäfer (UPV/EHU)
- **Strongly coupled plasmon-exciton hybrid nanostructures**  
Author: Emilie Dupont  
Supervisor: Marek Grzelczak (CFM) and Yury Rakovich (CFM)
- **Chemiluminescent single-chain nanoparticles for sensing cobalt ions**  
Author: Andrea Aguirre Baños  
Supervisors: José A. Pomposo Alonso (CFM) and María Ester Verde Sesto (CFM)
- **Endowing single-chain nanoparticles with fluorescent and drug delivery properties**  
Author: Arianne Encinar Manzano  
Supervisors: José A. Pomposo Alonso (CFM) and María Ester Verde Sesto (CFM)
- **Towards the development of novel bicolor sensor for neutrino detection**  
Author: Lander Murillo Lekuona  
Supervisors: Celia Rogero Blanco (CFM)
- **Real-time manipulation of optical trap with deformable mirror**  
Author: Harriet Kumi  
Supervisor: Gabriel Molina Terriza (CFM)

- **Charge-density-wave transition in VSe<sub>2</sub> from first principles**  
Author: Josu Diego López  
Supervisor: Ion Errea Lope (CFM)
- **Development of smart substrates for enhancing in near-field spectroscopy**  
Author: Alba Viejo Rodríguez  
Supervisor: Rainer Hillenbrand (CIC nanoGUNE)
- **Electron quantum transport in generic tight-binding models**  
Author: Andrés Felipe Bejarano Sánchez  
Supervisor: Thomas Frederiksen (DIPC)

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

- **Proximity effects in superconductor-ferromagnetic insulator bilayers of arbitrary thickness**  
Author: Maxime Infuso  
Supervisor: F. Sebastián Bergeret Sbarbaro (CFM)
- **Synthesis of poly(methacrylic-co-polyethylene glycol methacrylate) copolymers and its application on cementitious formulations**  
Author: Sara Pavo Belderrain  
Supervisors: José Ramón Leiza (Polymat, UPV/EHU) and Jorge Sánchez Dolado (CFM)
- **Tailoring the electronic properties of graphene nanoribbons by chemical substitution**  
Author: Iñigo Delgado Enares  
Supervisors: Daniel Sánchez Portal (CFM) and Aran García-Lekue (DIPC)



# UNDERGRADUATE EDUCATION PROGRAM

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## COURSES

In addition to the Master's and PhD programs, the staff at CFM also participates in a variety of undergraduate courses in 4 Faculties and University Schools of the University of the Basque Country (UPV/EHU). In total, more than 1400 teaching hours spread over 6 undergraduate degrees and 3 Master degrees at UPV/EHU are delivered by CFM staff.

## END OF COURSE PROJECTS AND SHORT STAY VISITS

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

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

## INTERNSHIPS

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

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



# WORKSHOPS, CONFERENCES AND SEMINARS

Despite the sanitary emergency, CFM scientists organized or co-organized 9 international workshops and conferences during 2020, out of which 6 had to be finally cancelled. Many of these meetings have been historically held in close cooperation with the Donostia International Physics Center (DIPC) foundation, which is an example of the excellent results brought by the synergistic collaboration between both institutions. These activities improve dramatically the impact and relevance of the individual and groups' research outcome.

Moreover, CFM researchers regularly give Invited and Plenary talks in international conferences, showing their leadership in their respective fields. Again, this activity was dramatically affected by the COVID19 crisis.

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



Auditorium

## Total Energy and Force Methods 2020

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

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

8-10/01/2020

## Software Carpentry Workshop

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

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

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

14, 15, 16 and 23/01/2020

## RSC Statistical Mechanics and Thermodynamics Group

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

Online

08/2020 (ongoing series)

# PhD SEMINAR SERIES

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

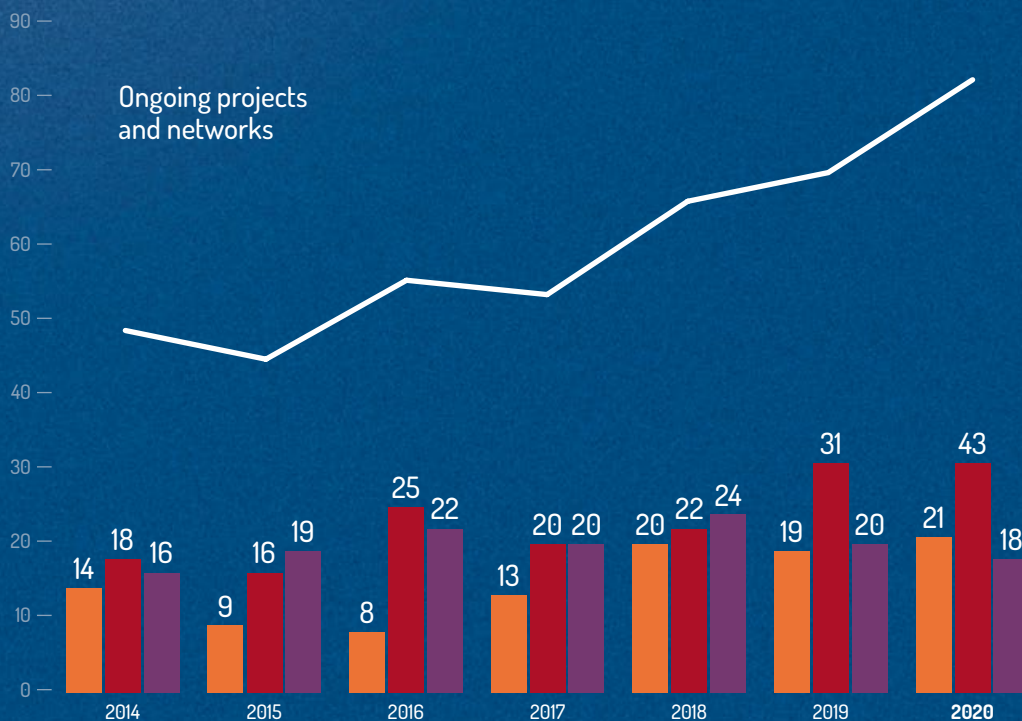
- **Study of the coadsorption of (O, CO) on Ru(0001)**  
Auguste Tetenoire  
22/01/2020
- **Transition-metal oxide chains: spin phases, magnetic anisotropy and coupling**  
Joseba Goikoetxea Perez  
22/01/2020
- **Mean field Hubbard method for non-equilibrium electron transport**  
Sofia Sanz Wuhl  
19/02/2020
- **Kerker conditions in lossless, absorption and optical gain regimes**  
Jorge Olmos Trigo  
19/02/2020
- **Fluorescent single-chain polymer nanoparticles based on Aggregation-Induced Emission (AIE) molecules**  
Julen de la Cuesta Leone  
11/03/2020
- **Synthesis and characterization of cyclic poly(glycidyl phenyl ether) with controlled dipolar microstructure**  
Jordan Ochs  
11/03/2020
- **Symmetry-protection of multiphoton states of light**  
Jon Lasa Alonso  
28/05/2020
- **Isolating Mie resonances in a dielectric sphere using angular momentum beams**  
Martín Molezuelas Ferreras  
28/05/2020

## MORE SEMINARS HOSTED BY CFM

- **Taming complex fluids with external fields**  
Fernando Bresme  
07/02/2020
- **Sub-Terahertz Spin Pumping from an Insulating Antiferromagnet**  
Enrique del Barco  
11/02/2020
- **Atomic-scale spin-sensing with a single molecule at the apex of a scanning tunneling microscope**  
Benjamin Verlhac  
20/02/2020
- **The polar surfaces of the delafossite oxides: from massive Rashba spin-splittings to itinerant surface ferromagnetism**  
Federico Mazzola  
09/03/2020
- **Computational Modelling of Metal-Organic Frameworks**  
Rémi Pétuya  
17/09/2020
- **Biological processes at cellular membranes - New knowledge through the use of neutron and X-ray Scattering**  
Marité Cárdenas  
18/11/2020
- **Porous materials at nanoscale - A neutron scattering insight**  
Margarita Russina  
24/11/2020
- **Nuclear Quantum effects enter the mainstream**  
Matthew Krzystyniak  
30/11/2020
- **Tailoring the interfacial assembly and the mechanical response of colloidal and biological systems**  
Armando Maestro  
02/12/2020
- **Neutron scattering and complementary investigations of fullerene solutions and polymer nanocomposites thin films**  
Timur Tropin  
04/12/2020

# COMPETITIVE FUNDING FOR RESEARCH PROJECTS

RESEARCH PROJECTS AND NETWORKS	Competitive public fundraising in 2020
<span style="color: orange;">■</span> BASQUE	415 644,34 €
<span style="color: red;">■</span> SPANISH	1 522 011,31 €
<span style="color: purple;">■</span> INTERNATIONAL	1 926 522,85 €
MPC-BERC	1 224 640,00 €
<b>— TOTAL</b>	<b>5 088 818,50 €</b>



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

# BASQUE RESEARCH PROJECTS AND NETWORKS

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- **EJ/GV, EKIZIEN 2019: Adquisición Equipamiento Científico, EC19-27**  
Recycling preparative SEC/GPC  
PI: Josetxo Pomposo Alonso
- **EJ/GV, ELKARTEK 2018, KK-2018/00001**  
nG8 - Investigación colaborativa para la caracterización avanzada de sistemas macroscópicos en la nanoescala  
PI: Javier Aizpurua Iriazabal
- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1182-19**  
Grupo de Espectroscopía Láser y Materiales Fotónicos  
PI: Rolindes Balda de la Cruz
- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1260-19**  
Desarrollo de nuevas metodologías en problemas destacados de Física de la Materia Condensada  
Partners: Ion Errea Lope; Aitor Bergara Jauregui
- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1255-19**  
Nanophysics Lab San Sebastián: desde la ciencia de superficies a los dispositivos  
PI: Enrique Ortega Conejero
- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1164-19**  
Q-NANOFOT - Nanofotónica cuántica para la caracterización de nuevos procesos y aplicaciones en espectroscopías moleculares, microscopía de campo cercano y tecnologías cuánticas con fotones  
PI: Javier Aizpurua Iriazabal  
co-PI: Nerea Zabala Unzalu
- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1246-19**  
Grupo de Fisicoquímica de Superficies y Nanoestructuras  
PI: Iñaki Juaristi Olliden
- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1175-19**  
PSMG - Polymers & Soft Matter  
PI: Juan Colmenero de León

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- **EJ/GV, IKERTALDE 2019, Grupo Consolidado IT1249-19**  
FunTheMaS – Fundamental Theoretical Materials Science  
co-PI: Ángel Rubio Secades
  - **EJ/GV, Proyectos de Investigación Básica y/o Aplicada 2018-2020 (PIBA), PIBA2018\_1\_0024**  
Diseño, elaboración y caracterización de materiales nano-micro estructurados ópticamente activos en el rango visible e infrarrojo próximo para la construcción de una fuente láser aleatoria de baja coherencia para aplicaciones biomédicas  
PI: Rolindes Balda de la Cruz
  - **EJ/GV, Proyectos de Investigación Básica y/o Aplicada 2020-2022 (PIBA), PIBA2020\_1\_0017**  
Hacia la computación cuántica topológica manipulando átomos en superconductores  
PI: Deungjang Choi
  - **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa Cooperera 2018, 2018 IZEN-000013**  
ELLAS INVESTIGAN IV: Afrikar emakumezko ikertzaile batek egonaldi bat egin dezan MPCn / ELLAS INVESTIGAN IV: Estancia de investigación en el MPC de una investigadora africana
  - **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa Cooperera 2019, 2019-IZEN-02**  
ELLAS INVESTIGAN V: Afrikar emakumezko ikertzaile batek egonaldi bat egin dezan MPCn / ELLAS INVESTIGAN V: Estancia de investigación en el MPC de una investigadora africana
  - **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, Gipuzkoa Cooperera 2020, 2020-IZEN-000012-01**  
ELLAS INVESTIGAN VI: Afrikar emakumezko ikertzaile batek egonaldi bat egin dezan MPCn / ELLAS INVESTIGAN VI: Estancia de investigación en el MPC de una investigadora africana

# BASQUE RESEARCH PROJECTS AND NETWORKS

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- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2019 RED2019, 2019-CIEN-000003-01**

Desarrollo de nanopartículas poliméricas unimoleculares conteniendo metales divalentes como catalizadores para la síntesis de aditivos usados en la preparación de biodiesel

PI: Josetxo Pomposo Alonso

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2019 RED2019, 2019-CIEN-000050-01**

Síntesis química de materiales nanoestructurados para salud y energía

PI: Yury Rakovich

- **Gipuzkoako Foru Aldundia/Diputación Foral de Gipuzkoa, SAREA2020 RED2020, 2020-CIEN-000009-01**

Estudio de materiales fotovoltaicos de última generación mediante técnicas neutrónicas, microscopía y espectroscopia túnel, y cálculos de primeros principios

PI: Félix Fernández Alonso

- **Biozientziak Gipuzkoa Fundazioa, Convocatoria de Proyectos de I+D+i COVID-19**

DETENTE SARS - Detección mediante técnicas físico-químicas específicas y ultrasensibles de SARS-CoV-2

PI: Celia Rogero Blanco

- **UPV/EHU, Azpiegitura Zientifikoa/Infraestructura Científica 2020, INF 20/03**

Reómetro rotacional para polímeros y materia blanda

PI: Juan Colmenero de León

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

Polímeros y materiales avanzados: Física, química y tecnología

PI: Iñaki Juaristi Oñden

- **UPV/EHU, Ikerketa Taldeak/Grupos de Investigación UPV/EHU 2017, GIU17/014**

Grupo de Espectroscopía Láser y Materiales Fotónicos

PI: Rolindes Balda de la Cruz



# SPANISH RESEARCH PROJECTS AND NETWORKS

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- **Proyectos I+D Fundamental (Excelencia) 2016, FIS2016-76617-P**  
Excitaciones electrónicas en superficies y nanoestructuras  
PI: Andrés Ayuela Fernández
- **Proyectos I+D Fundamental (Excelencia) 2016, FIS2016-77188-P**  
Teoría y simulación de fenómenos ópticos y de transporte en materiales girotrópicos  
PI: Ivo Souza
- **Retos Colaboración 2016, RTC-2016-5681-7**  
SIESTA pro – Spanish initiative for electronic simulations with thousands of atoms: Código abierto con garantía y soporte profesional  
PI: Daniel Sánchez Portal
- **Retos Investigación 2016, MAT2016-78293-C6-4-R**  
Teoría de nanoestructuras moleculares funcionales para dispositivos optoelectrónicos  
PI: Daniel Sánchez Portal
- **Retos Investigación 2016, MAT2016-78293-C6-5-R**  
FunMolDev-Nanoestructuras moleculares funcionales para dispositivos optoelectrónicos: Guiando reacciones en superficies  
PI: Celia Rogero Blanco
- **Proyectos I+D Fundamental (Excelencia) 2017, FIS2017-82804-P**  
Transporte electrónico en estructuras híbridas: materiales de baja dimensionalidad, superconductores, materiales magnéticos, semiconductores y metales normales  
PI: Sebastián Bergeret Sbarbaro  
co-PI: Dario Bercioux (DIPC, Ikerbasque)
- **Proyectos I+D Fundamental (Excelencia) 2017, FIS2017-87363-P**  
Nanofotónica cuántica: explorando las correlaciones cuánticas de los fotones usando nanopartículas  
PI: Gabriel Molina Terriza

# SPANISH MINISTRY RESEARCH PROJECTS AND NETWORKS

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- **Proyectos I+D Fundamental (Excelencia) 2017, MAT2017-88374-P**  
Magnetismo exótico y fenómenos de correlación de electrones en la superficie y el sólido de materiales basadas en tierras raras  
PI: Frederik Michael Schiller  
Co-PI: Denis Vyalikh (DIPC, Ikerbasque)
- **Proyectos I+D Fundamental (Excelencia) 2017, MAT2017-87035-C2-2-P**  
Vidrios y vitrocerámicos dopados con tierras raras para aplicaciones fotónicas  
PI: Rolindes Balda de la Cruz
- **Retos Investigación 2017, MAT2017-88377-C2-2-R**  
Transistores de spin basados en heteroestructuras Van der Waals  
PI: Sara Barja Martínez  
co-PI: Miguel Moreno Ugeda (DIPC, Ikerbasque)
- **Redes de Excelencia 2017, MAT2017-90771-REDT**  
ESpín - Red: Red Española de Espintrónica  
Partner: Andrés Arnau Pino
- **Contratos Personal Técnico de Apoyo (PTA) 2017, PTA2017-14359-I**  
Técnico para el laboratorio de rayos X del CFM (CSIC-UPV/EHU):  
mantenimiento del servicio y explotación de nuevas oportunidades de los equipos  
Lab Technician: Amaia Iturrospe Ibarra  
Supervisor: Arantxa Arbe Méndez
- **Contratos Ramón y Cajal (RyC) 2017, RYC-2017-21931**  
Novel physical phenomena in two-dimensional materials  
PI: Sara Barja Martínez
- **Contratos Juan de la Cierva – Incorporación (JdC-I) 2017, IJCI-2017-31600**  
Polymers and Soft Matter: Nanostructures and physical properties at the nanoscale  
PI: Daniel Enrique Martínez Tong  
Supervisor: Ángel Alegría Loinaz
- **Proyectos de I+D+i Retos Investigación 2018 (RTI2018), RTI2018 097895 B C44**  
FUN-SOC - Novel Functionalities Driven by Spin-Orbit Interactions  
PI: Nicolás Lorente Palacios  
Co-PI: Deungjang Choi

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- **Proyectos de I+D+i Retos Investigación 2018 (RTI2018), RTI2018 098554 B I00**  
**E-CRETE - Energy storage solutions based on ConCRETE**  
PI: Jorge Sánchez Dolado  
Co-PI: Juan José Gaitero Redondo (Tecnalia)
  - **Proyectos de I+D+i de Generación de Conocimiento 2018 (PGC2018), PGC2018-094548-B-I00**  
**SONIBOND - Tailored Soft Nano-Objects Based on Intrachain Bonding: From Design to Materials**  
PI: Ángel Moreno Segurado  
Co-PI: Josetxo Pomposo Alonso
  - **Redes Investigación 2018 - Red Temática, RED2018-102752-T**  
**NANOLIGHT.es - Light Control on the Nanoscale**  
PI: Javier Aizpurua Iriazabal
  - **Redes Investigación 2018 - Red Temática, RED2018-102833-T**  
**OSMolSis - Ciencia Molecular en Superficies: Síntesis y Funcionalidad**  
PI: Daniel Sánchez Portal
  - **Redes Investigación 2018 - Red Temática, RED2018-102459-T**  
**CAT&SCALE - (Photo-)Electrocatalysis: from the Atomic Scale to Advanced Devices**  
PI, Network Coordinator: Sara Barja Martínez
  - **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-104650GB-C21**  
**Dinámica en soluciones acuosas de polímeros y biopolímeros (subproyecto coordinador)**  
**Proyecto Coordinado: BRIDGE - Cerrando la brecha entre los polímeros sintéticos y los biopolímeros - propiedades físicas y químicas**  
PI: Silvina Cervený Murcia  
Co-PI: Gustavo A. Schwartz Pomeraniec
  - **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-107396GB-I00**  
**GASOLIN - Interfaces gas/sólido: acoplamiento entre la dinámica nuclear y la dinámica electrónica**  
PI: Maite Alducin Ochoa  
Co-PI: Ricardo Díez Muiño

# SPANISH MINISTRY RESEARCH PROJECTS AND NETWORKS

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- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-105488GB-I00**  
2EDiSNa - Excitaciones electrónicas y dinámicas en superficies y nanoestructuras  
PI: Andrés Ayuela Fernández  
Co-PI: Silkin Vyacheslav (DIPC, Ikerbasque)
- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-107432GB-I00**  
QUATOPHOT - Estudio de los efectos cuánticos en nanofotónica a escala atómica  
PI: Javier Aizpurua Iriazabal  
Co-PI: Rubén Esteban Llorente
- **Proyectos de I+D+i de Generación de Conocimiento 2019 (PGC2019), PID2019-103910GB-I00**  
VIMAGSOC - Vibraciones y magnetismo en sistemas nanoscópicos con acoplamiento spin-órbita  
PI: Andrés Arnau Pino  
Co-PI: Asier Eiguren Goyenechea (UPV/EHU)
- **Proyectos de I+D+i de Retos Investigación 2019 (RTI2019), PID2019-111772RB-I00**  
QUATH - Análisis cuantitativo de la contribución de cargas calientes y efecto térmico en fotocatalisis asistida por efecto plasmónico  
PI: Marek Grzelczak  
Co-PI: Jon Mattin Matxain Beraza (UPV/EHU)
- **Proyectos de I+D+i de Retos Investigación 2019 (RTI2019), PID2019-107338RB-C63**  
FunMolSys - Síntesis en Superficie de Sistemas Moleculares Funcionales (subproyecto)  
Proyecto Coordinado: MONOMET - Transferencia de sistemas moleculares funcionales a superficies no metálicas  
PI: Martina Corso  
Co-PI: Dimas García de Oteyza Feldermann (DIPC, Ikerbasque)

- 
- **Proyectos de I+D+i de Retos Investigación 2019 (RTI2019), PID2019-107338RB-C66**  
TheoFunMolSys - Teoría de propiedades electrónicas, topológicas, magnéticas y vibracionales de nanoSistemas Moleculares Funcionales (subproyecto)  
Proyecto Coordinado: MONOMET - Transferencia de sistemas moleculares funcionales a superficies no metálicas  
PI: Daniel Sánchez Portal  
Co-PI: Arantzazu García Lekue (DIPC, Ikerbasque)
  - **Contratos Personal Técnico de Apoyo (PTA) 2019, PTA2019-018134-I**  
Apoyo técnico de los laboratorios de ultra-alto vacío del Centro de Física de Materiales (CFM)-Centro Mixto CSIC-UPV/EHU  
Lab Technician: Laura Fernández Gómez-Recuero  
Supervisor: Martina Corso
  - **Adquisición de Equipamiento Científico-Técnico 2019, EQC2019-005735-P**  
Installation of a liquid Helium recovery and supply plant for cryogenic experimental systems  
PI: Martina Corso
  - **Acciones de Dinamización Europa Excelencia 2020, EUR2020-112116**  
ARTS - Atomic research for topological superconductors / Investigación atómica para superconductores topológicos  
PI: Deungjang Choi
  - **Acciones de Dinamización Europa Excelencia 2020, EUR2020-112066**  
ReversO<sub>2</sub> - Oxygen conversion reactions: Fundamental insights for rational design  
PI: Sara Barja Martínez
  - **CSIC, I-LINK+ 2018, Red de Internacionalización, LINKB20012**  
NEXTWATER-ilink - Network Exchanges Training program on dynamics and nanostructure of biomolecules in WATER solutions  
PI: Silvina Cervený Murcia
  - **CSIC, Fondo de Apoyo a los Servicios Científico Técnicos (FAS) 2019, FAS\_19\_0297**  
Servicio científico-técnico Centro de Cálculo de Altas Prestaciones - Mejora del sistema de climatización del Centro de Proceso de Datos 2 (CPD-2)

# SPANISH MINISTRY RESEARCH PROJECTS AND NETWORKS

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- **CSIC, Programa de Apoyo a la Infraestructura (PAI) 2019-2020, PAI 06-3356**  
Implementación del nuevo laboratorio de síntesis
- **CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2019, 2019AEP061**  
Teoría de nanoestructuras moleculares funcionales para dispositivos optoelectrónicos  
PI: Daniel Sánchez Portal
- **CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2019, 2019AEP062**  
Nanoestructuras moleculares funcionales para dispositivos optoelectrónicos: Guiando reacciones en superficies  
PI: Martina Corso
- **CSIC, Ayuda Extraordinarias para la Preparación de Proyectos en el Marco del Plan Estatal de I+D+i 2019, 2019AEP042**  
Excitaciones electrónicas en superficies y nanoestructuras  
PI: Andrés Ayuela Fernández
- **CSIC, I-LINK+ 2019, Colaboración Científica Internacional, LINKC20002**  
On-surface polymerization for high performance (opto)electronics  
PI: Martina Corso
- **CSIC, I-COOP+ 2019, Cooperación Científica para el Desarrollo, COOPB20432**  
Diluted magnetic quantum dots assemblies for innovative spintronics  
PI: Martina Corso
- **CSIC, Fondo de Apoyo a los Servicios Científico-Técnicos (FAS) 2020, FAS2020\_058**  
Unidad de control para TPS SPECTRA 3000
- **CSIC, Fondo de Apoyo a los Servicios Científico-Técnicos (FAS) 2020, FAS2020\_059**  
Sistema de refrigeración para TPS SPECTRA 3000
- **CSIC, Programa de Apoyo a la Infraestructura (PAI) 2020-2021, PAI2020\_4026**  
Adecuación de laboratorios de ciencia de superficies del CFM

# EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

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- **ERC Advanced Grant (ERC-2015-AdG), GA 694097**  
QSpec-NewMat - Quantum Spectroscopy: exploring new states of matter out of equilibrium  
PI: Ángel Rubio Secades
- **INFRAIA: Integrating Activities for Advanced Communities (H2020 INFRAIA-2016-1), GA 731019**  
EUSMI - European infrastructure for spectroscopy, scattering and imaging of soft matter  
PI: Ángel Alegría Loinaz
- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN 01-2016-2017), GA 766864**  
MEMO-Mechanics with Molecules  
PI: Nicolás Lorente Palacios
- **INTERREG (ETC) V A: Cross-border Cooperation, POCTEFA 2014-2020, EFA194/16/TNSI**  
TNSI-Trans-Pyrenean Node for Scientific Instrumentation  
PI: Celia Rogero Blanco
- **INTERREG (ETC) V C: Interregional Cooperation, Aquitania-Euskadi-Navarre Euroregion Projects 2017**  
DINaMO-FiVe - Durabilidad de Infraestructuras en ambiente marino: Nano-Materiales Optimizados como Fibras Verdes  
PI: Silvina Cervený Murcia
- **Setting up European or International Scientific Networks (Montage de Réseaux Scientifiques Européens ou Internationaux, MRSEI) Instrument, ANR-18-MRS1-0014**  
NaWaGui - Nanostructured Waveguides for Photonics  
PI: Rolindes Balda de la Cruz
- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN 01-2016-2017), GA800923**  
SUPERTED - Thermoelectric detector based on superconductor-ferromagnet heterostructures  
PI: Sebastián Bergeret Sbarbaro  
Co-PI: Celia Rogero Blanco

# EUROPEAN AND INTERNATIONAL RESEARCH PROJECTS AND NETWORKS

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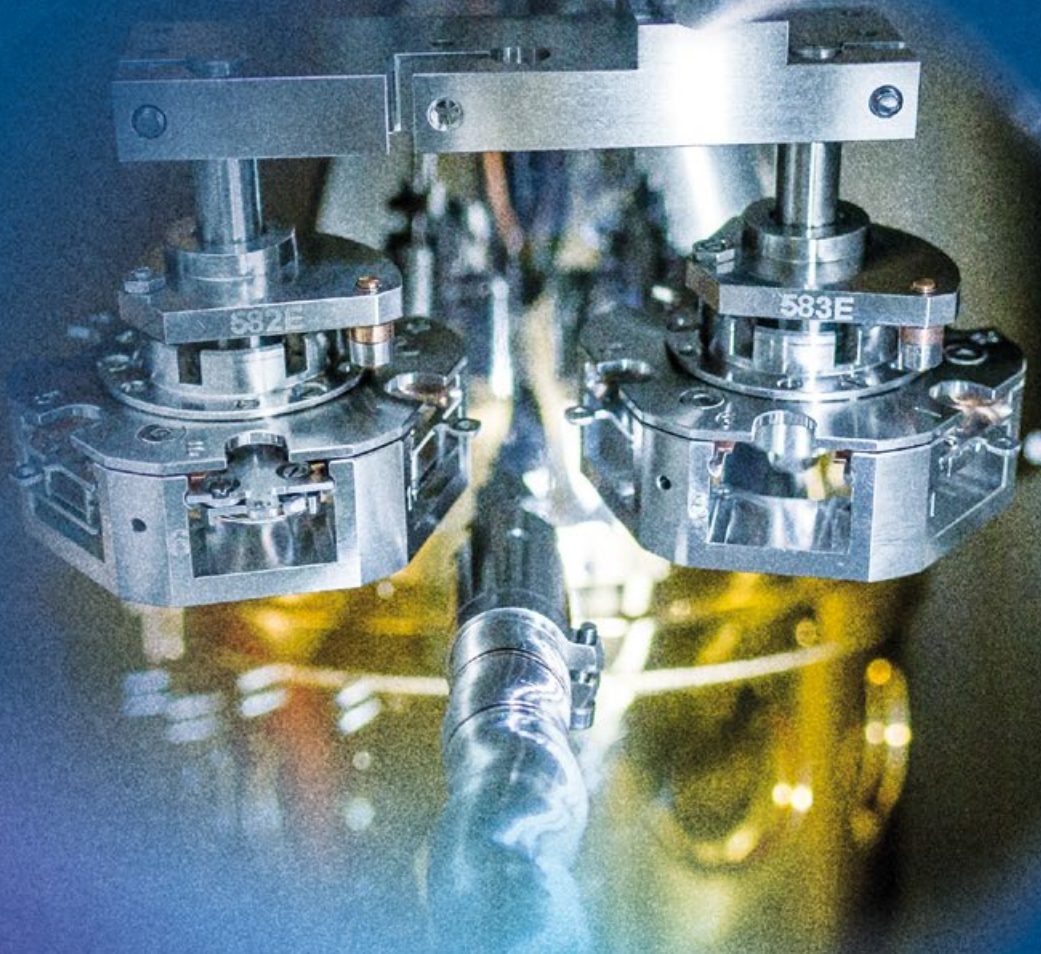
- **NMBP: Nanotechnologies, Advanced Materials, Biotechnology, and Advanced Manufacturing and Processing, Innovative solutions for the Conservation of 20th Century Cultural Heritage (H2020-NMBP-35-2017), GA 760858**  
InnovaConcrete - Innovative materials and techniques for the conservation of 20th century concrete-based cultural heritage  
PI: Jorge Sánchez Dolado
- **COST Action 2017, CA17139**  
EUTOPIA - European Topology Interdisciplinary Action  
Management Committee Member: Ángel Moreno Segurado
- **Marie Curie Individual Fellowship (H2020-MSCA-IF-2017), GA 797109**  
MagicFACE - Magnetic hybrid metal-organic interfaces  
Supervisor: Enrique Ortega Conejero
- **ERC Starting Grant (ERC-2018-STG), GA 802533**  
SuperH - Discovery and characterization of hydrogen-based high-temperature superconductors  
PI: Ion Errea Lope
- **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN 01-2018 2019 2020), GA 829067**  
THOR - TeraHertz detection enabled by mOleculaR optomechanics  
PI: Javier Aizpurua Iriazabal
- **Leadership in Enabling and Industrial Technologies, Space (H2020 SPACE 11 TEC-2018), GA 821932**  
SMART-FLEX - Next generation metamaterial-based SMART and FLEXible optical solar reflectors  
PI: Javier Aizpurua Iriazabal
- **EIG CONCERT-Japan: 5th Joint Call, Functional Porous Materials, PCI2019 103657**  
PoroPCM - Functional POROUs cementitious nanocomposites for heat storage in buildings using Phase Change Materials  
PI: Jorge Sánchez Dolado



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- **Marie Curie Individual Fellowship (H2020-MSCA-IF-2018), GA 839237**  
**PhotoWann - Bulk Photovoltaic effect via Wannier functions**  
Supervisor: Ivo Souza
  - **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN-01-2018-2019-2020), GA 861980**  
**POSEIDON - NanoPh0tonic devices applying SElf-assembled colloIDs for novel ON-chip light sources**  
PI: Javier Aizpurua Iriazabal
  - **FET-OPEN: Novel Ideas for Radically New Technologies (H2020 FETOPEN-01-2018-2019-2020), GA 863170**  
**ArtiBLED - Engineered Artificial Proteins for Biological Light-Emitting Diodes**  
PI: Pedro Braña Coto
  - **NMBP: Integration of Energy Smart Materials in non-Residential Buildings, LC-EEB-01-2019 (H2020-NMBP-EEB-2019), GA 870114**  
**NRG-Storage - integrated porous cementitious Nanocomposites in non-Residential building envelopes for Green active/passive energy STORAGE**  
PI: Jorge Sánchez Dolado



# TRANSFER OF KNOWLEDGE



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

The portfolio of contracts and collaboration agreements with different companies or external parties has been very productive during 2020. Some examples of the partners involved are:



#### Janssen Research (Belgium)

Study of dielectric properties of polymers



#### Basque Culinary Center Fundazioa

Food science. Physico-chemical properties of complex materials



#### Mugaritz

Gastronomy and food science



#### SIMUNE ATOMICS L.T.D.

Development of software tools to improve the capabilities and the analysis of data computed with the SIESTA/TranSIESTA package



#### Považská cementáreň (Slovakia)

Study of hydrated cement pastes



#### Baskrete cross-border initiative

Concrete science and technology



#### Michelin (France)

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



#### Mujeres por África Foundation

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



#### Kutxa Fundazioa

Scientific cultural activities

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

# SCIENCE AND SOCIETY

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

Developing a so-called "scientific culture" in the public has become crucial these days. In this major task, all the members of the scientific community have a role to play, starting from the institutions and including tenured scientists, post-doctoral researchers, pre-doctoral researchers and science communicators.



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

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

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

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

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

#scienceandsociety

# SCHOOL VISITS

Since 2013, together with the Donostia International Physics Center (DIPC), CFM has carried out a program of visits where both centers open their doors to high school students, approximately every two weeks during the academic year.

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

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

# EMAKUMEAK ZIENTZIAN 2020

[emakumeakzientzian.eus](http://emakumeakzientzian.eus)

7-14/02/2020

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

## SCIENCE IS INDEED A GIRLS' THING

In order to achieve access and full and equal participation in science for women and girls, in 2016 the United Nations General Assembly decided to proclaim 11 February as International Women's and Girls' in Science Day.

To commemorate this day, CFM and CIC nanoGUNE co-ordinated the program that brings together the activities of 9 research centers and science-related institutions in the Donostia / San Sebastián area, to make visible the activity of women in science, and to break with the typically masculine roles attributed to scientific-technical activities and encourage the choice of scientific careers among girls and adolescents.

In an unprecedented collaboration, with more than 60 volunteers onboard, the 9 centers joined forces to present a full week program that aimed teenager women, school kids, elder women (above 55), citizens in general and the scientific community.



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

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



482

Participants

60

Volunteers

9

Entities

51

Impacts in Media

2 881 500

Estimated Audience

16 368,11 €

Contributions

## THE “EMAKUMEAK ZIENTZIAN” INITIATIVE WAS RECOGNIZED WITH THE STEAM EUSKADI SEAL

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



# “QUÉ SABEMOS DE...” TALK SERIES

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

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

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

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



Available at CFM's  
YouTube channel or  
scanning this code

- **Nuevos Coronavirus: Inesperados compañeros de viaje**

**Isabel Sola (CNB-CSIC)**

Co-director of the Coronavirus Laboratory of the National Biotechnology Centre, CNB-CSIC

- **Creando nuevos materiales en la nanoescala**

**Martina Corso (CFM)**

CSIC Researcher at the Nanophysics Laboratory at CFM

- **La frontera de la física fundamental**

**Alberto Casas (CSIC-UAM)**

Doctor in Theoretical Physics and Research Professor at the Institute of Theoretical Physics (CSIC-UAM).

- **Biología con las herramientas CRISPR en los tiempos del coronavirus**

**Lluís Montoliu (CNB-CSIC y CIBERER-ISCI)**

CSIC and CIBERER-Carlos III Health Institute Researcher at the National Biotechnology Centre in Madrid.





# PRIDE IN STEAM DAY

[orgulloenciencia.dipc.org](http://orgulloenciencia.dipc.org)

ONLINE

18/11/2020

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

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

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



Available at CFM's  
YouTube channel or  
scanning this code

Javier Armentia  
(Chair)



Juani  
Bermejo-Vega



Mari Luz  
Cádiz



Daniel  
Martínez-Tong



Laura  
Muelas de Ayala



Marina  
Peña

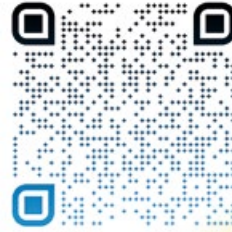
# LA CIENCIA SEGÚN FORGES

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

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

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

More than 2 000 attendees visited the exhibit.



Available at CFM's  
YouTube channel or  
scanning this code



# OUTREACH TALKS

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

## ORGANIZED BY CFM

### The world's smallest car race

**Nicolás Lorente (CFM) and Christian Joachim (founder of the NanoCar Race)**

29/01/2020

Kutzakultur Plaza (Tabakalera)

### El coronavirus y el futuro que nos espera (round table)

**Sara de La Rica, Eduardo Maíz y Juan Ignacio Pérez**

**Chairman: Aitor Bergara**

26/09/2020

Bidebarrieta Library

## II CURSO DE CULTURA CONTEMPORÁNEA

### Las ciencias y las humanidades en la cultura contemporánea

**Gustavo Ariel Schwartz**

16/10/2020

Online

## ZIENTZIAREN GILTZAK

Talks organized by *Zientziaren Giltzak* science community at Ondarroa

### Argia ttiki egiten denean

**Javier Aizpurua**

19/10/2020

Behikozini (Ondarroa)

## PRISMA CONFERENCE

### Outreach to get out there

**Idoia Mugica (CFM)**

16/11/2020

Online

## ZIENTZIA KUTXA

Talks organized by DIPC and *Kutxa fundazioa*

### Supereroankortasuna, markak hausten!

**Ion Errea**

29/05/2020

Online

## CINEMA AND SCIENCE

Cycle organized by DIPC and *Filmoteka Vasca*.

Presentation and discussion on the following movies:

### Agora

**Pedro Miguel Etxenike**

20/01/2020

Tabakalera (Donostia)

11/01/2020

Museum of Fine Arts of Bilbao

### Her

**Gustavo Ariel Schwartz**

06/02/2020

Tabakalera (Donostia)

08/02/2020

Museum of Fine Arts of Bilbao

### X: The man with X-Ray eyes

**Javier Aizpurua**

05/03/2020

Tabakalera (Donostia)

07/03/2020

Museum of Fine Arts of Bilbao

Outreach talk in the framework of the cycle:

### Herramientas de luz: de la ciencia ficción a las películas moleculares

**Nerea Zabala**

26/02/2020

Bidebarrieta Central Library

# ACTIVITY IN MASS MEDIA

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

Press articles

46\*

Radio

56

\*Scientific publications excluded

Online press

240\*

TV

13

Science, and particularly Material Physics Science, is presented in a simple and close language, in an effort to make scientific concepts and properties understandable and attractive to the general public.

An example of this intense activity is Ion Errea's collaboration with *Udako Faktoria* program that continued throughout the summer on a weekly basis, and the permanent section "Breakfast with Science" in the *Goiz Kronika* program of *Euskadi Irratia*, run every Sunday by Idoia Mugica, head of communication and dissemination of CFM. In addition to this, since September 2020 every two weeks Idoia Mugica presents a science section in the daily TV show "Eztabaidan" in the Basque Public Television (ETB1).

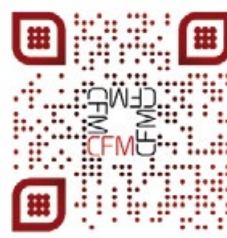
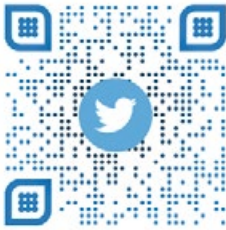
Many researchers were invited to participate in debates, interviews or articles in the general press. Television programs such as "Ur Handitan" (ETB1) or "Teknopolis" (ETB1/ETB2) focused on science and particularly on the CFM and its researchers.



# @CFMDONOSTIA

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



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

Users can [subscribe to CFM's mail list](#) to be updated on the information about the activities and events organized at CFM and stay tuned following us in our social media channels.



# OUTREACH COLLABORATION NETWORK

CFM has established strategic alliances regarding scientific outreach initiatives which create important synergies. These are the CFM's main partners in this strategy:

Universidad del País Vasco /  
Euskal Herriko Unibertsitatea



Consejo Superior de Investigaciones  
Científicas



Donostia International  
Physics Center



CIC nanoGUNE



CIC biomaGUNE



Polymat



Biodonostia



Tecnun



Ceit



Elhuyar



Eureka! Zientzia Museoa



Pride in STEM



PRISMA



Pint of Science



Aulas Kutxa – kutxakultur



FECYT



Diputación Foral de Guipúzcoa /  
Gipuzkoako Foru Aldundia



Fomento-Sustapena  
Donostia / San Sebastián



La Mecánica del Caracol  
(Radio Euskadi)



Goiz Kronika eta Udako  
Faktoria



Eztabaidan



Cátedra de Cultura  
Científica (UPV/EHU)



# GENDER EQUALITY & DIVERSITY AT CFM

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

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

The current GEC is composed by:

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

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

# PLAN IMPLEMENTATION OVERVIEW (2020-2024)

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

KEY AREA	OBJECTIVES	ACTIONS
Organizational culture	<ul style="list-style-type: none"> <li>• Create an inclusive organizational culture, with a gender-aware leadership and transparency at its core</li> <li>• Promote diversity and inclusivity with the institutional use of language (written and visual)</li> </ul>	<b>14</b>
A diverse workforce	<ul style="list-style-type: none"> <li>• Improve the gender balance at all work-positions and levels</li> <li>• Promote initiatives to support the career progression of the underrepresented gender to high and top positions</li> </ul>	<b>11</b>
Work-life balance	<ul style="list-style-type: none"> <li>• Develop a working environment that facilitates the combination of work, family and private life for women and men</li> </ul>	<b>6</b>
Sexual harassment at the working environment	<ul style="list-style-type: none"> <li>• Prevent and combat sexual and gender-based sexist harassment at CFM.</li> </ul>	<b>8</b>
Gender equality and research	<ul style="list-style-type: none"> <li>• Promote gender-aware research excellency within and outside CFM</li> <li>• Promoting gender diversity and inclusivity at congresses and conferences</li> </ul>	<b>5</b>



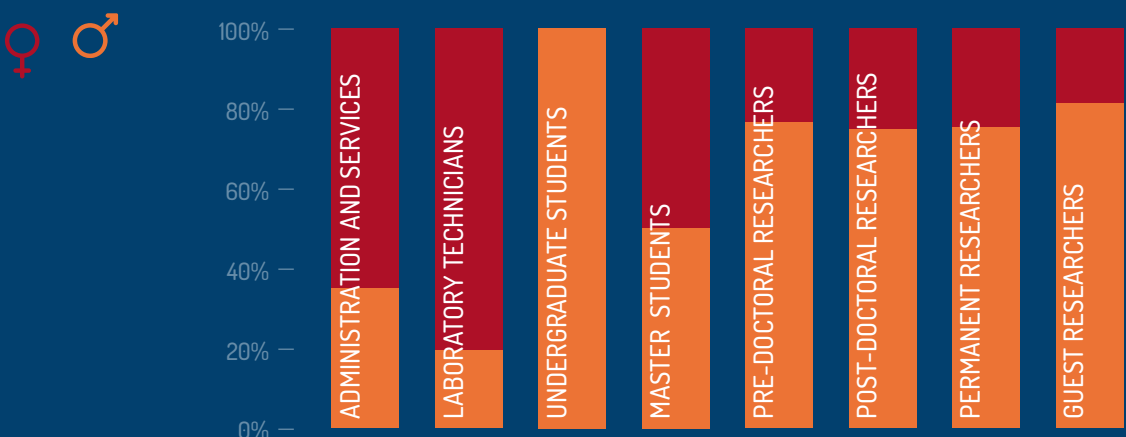
# DIAGNOSIS 2020

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

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

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

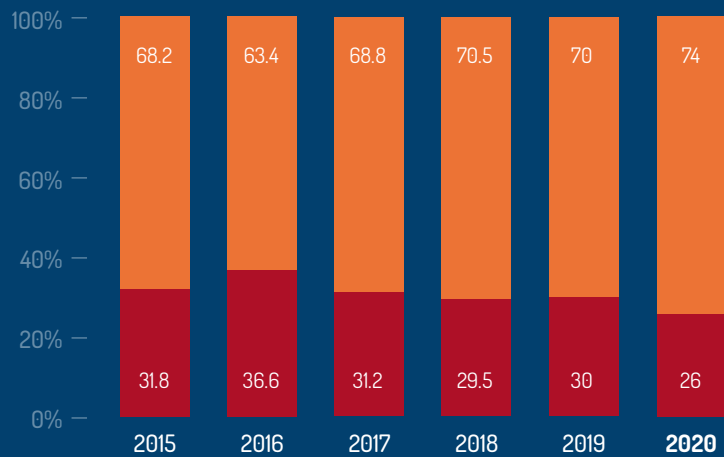
## Staff distribution at CFM according to category and gender (percentage)



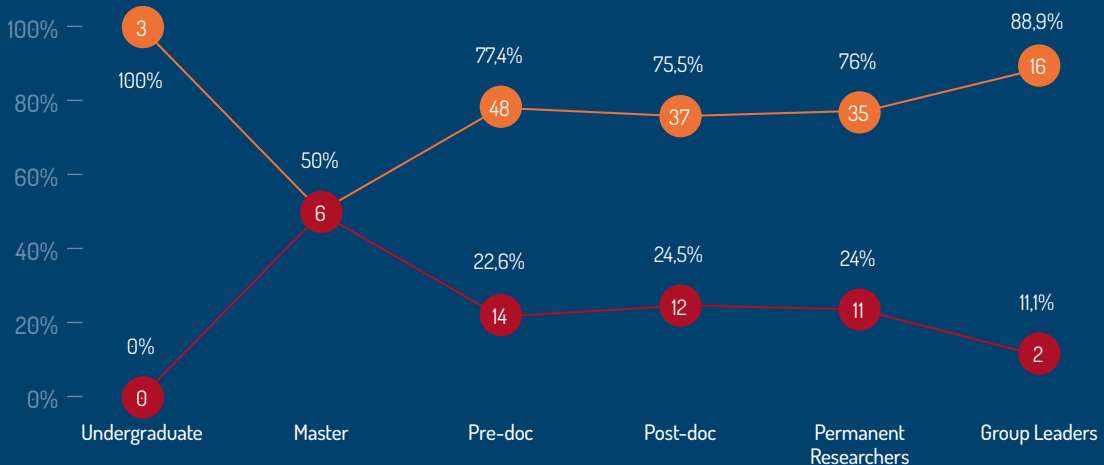
According to this data, the disproportion in the distribution of women/men in the center starts already at the earliest stage of the scientific career. Currently, less than 25% of the pre-doctoral researchers at CFM are women. The gender imbalance is accentuated as the responsibility for the job and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

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

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



### Distribution of CFM Scientific community in percentage by gender and position



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

## ACTIONS IN PLACE 2020

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When the CFM GEP was officially launched in October 2020, a series of specific actions to be addressed in the short term were already identified. The aim of those was, among other things, to inform and carry out activities to raise **awareness** of gender issues among the entire center's staff, as well as to the general public, and to **encourage scientific vocation in young women**.

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

In addition to this programs, specific actions like "Science by Women" or "Learn Africa" carried out together with Women for Africa Foundation and *Gipuzkoa Coopera*, show the commitment acquired so far (see *Miscellaneous* section of this report for further detail).

Nevertheless, it is worth mentioning that during 2020 CFM did also achieve:

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

# MISCELLA- NEOUS

## PHD RECRUITMENT FAIR 2020

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

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

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

## CFM AND WOMEN FOR AFRICA

### GIPUZKOA COOPERA PROGRAM WITH THE WOMEN FOR AFRICA FOUNDATION, DIPC, AND CFM

*Gipuzkoa Coopera* is a project launched by the Provincial Council of Gipuzkoa in 2017 and aims to promote development and cooperation by extending them to non-conventional activities. CFM has been part of the program since its very beginning, and the last three years it has materialized in a collaboration with the foundation Women for Africa.

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

Thanks to this initiative, in the framework of the program “Science by Women” promoted by the foundation Women for Africa, two African researchers would carry out six-month research stays at DIPC and CFM. The Provincial Council of Gipuzkoa financed each of these long stays with 25 000€. The female African researcher visiting and collaborating at CFM in 2019 and early 2020 was Dr. **Jetro Epse Njukeng Nkengafac** from Cameroon, who joined the Polymers and Soft Matter group, hosted by Prof. Ángel Alegría. However, her stay was interrupted by the health alert caused by COVID19.

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

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

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

### LEARN AFRICA

Together with the “Science by Women” program, the Women for Africa Foundation launches “Learn Africa”, an initiative that aims to promote the transfer of knowledge, exchange and training of undergraduate and graduate young African women students through scholarships in Spanish universities that collaborate in this initiative.

Since 2018, DIPC and CFM joined the program and offered a grant that fully covers the stay and expenses of a student to enroll in the Master in Nanoscience program of the UPV/EHU. In 2020, Harriet Kumi from Ghana, the recipient of the scholarship in 2019, finished and defended her Master Thesis at CFM under the supervision of Gabriel Molina at the Quantum Nanophotonics Lab.

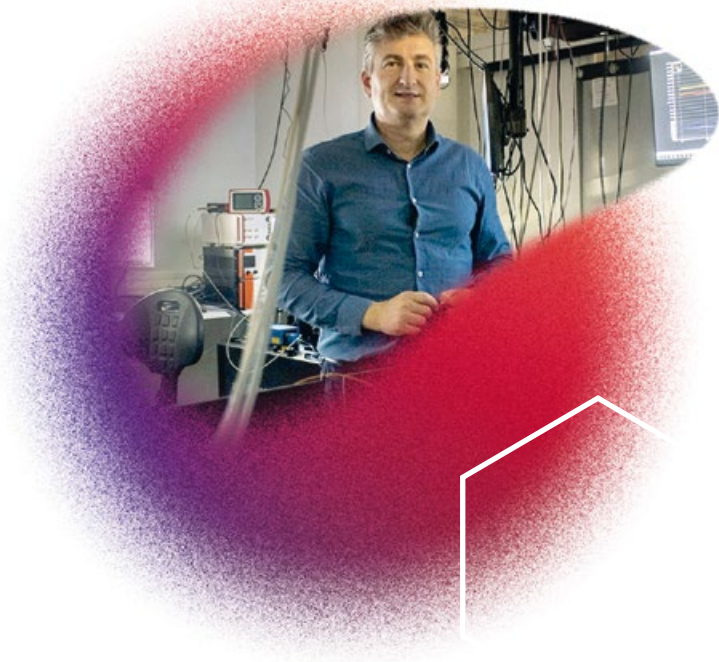


## HIGHLY CITED RESEARCHER 2020

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### PROF. JAVIER AIZPURUA IRIAZABAL

After being included for the first time in 2017, Professor Javier Aizpurua remained in the 2020 list of the most cited researchers in the world for the fourth year in a row, according to the database drawn up by Clarivate Analytics. Prof. Javier Aizpurua is head of the "Theory of Nanophotonics" group at CFM and DIPC. Highly cited researchers are acknowledged by the number of highly cited papers (in the top 1%) within an area (in this case, Physics), according to the database of "Web of Science" over the last eleven-year period.



## ERC GRANT FOR THE PHOTONOW PROJECT BY DR. JULEN IBAÑEZ

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



# THE SCIENCE OF CONCRETE THAT COULD WORK THE MIRACLE

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

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



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**cfm.ehu.es**

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

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Report Coordination: Idoia Mugica

Edition and corrections: Ioritz Paulis and Idoia Mugica

Photo/Picture credits: Ioritz Paulis and Javier Larrea

Design: batuta.eus