

REPORT 2013

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Materialen Fisika Zentroa
Centro de Física de Materiales
Materials Physics Center

ACTIVITY REPORT 2013

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CSIC

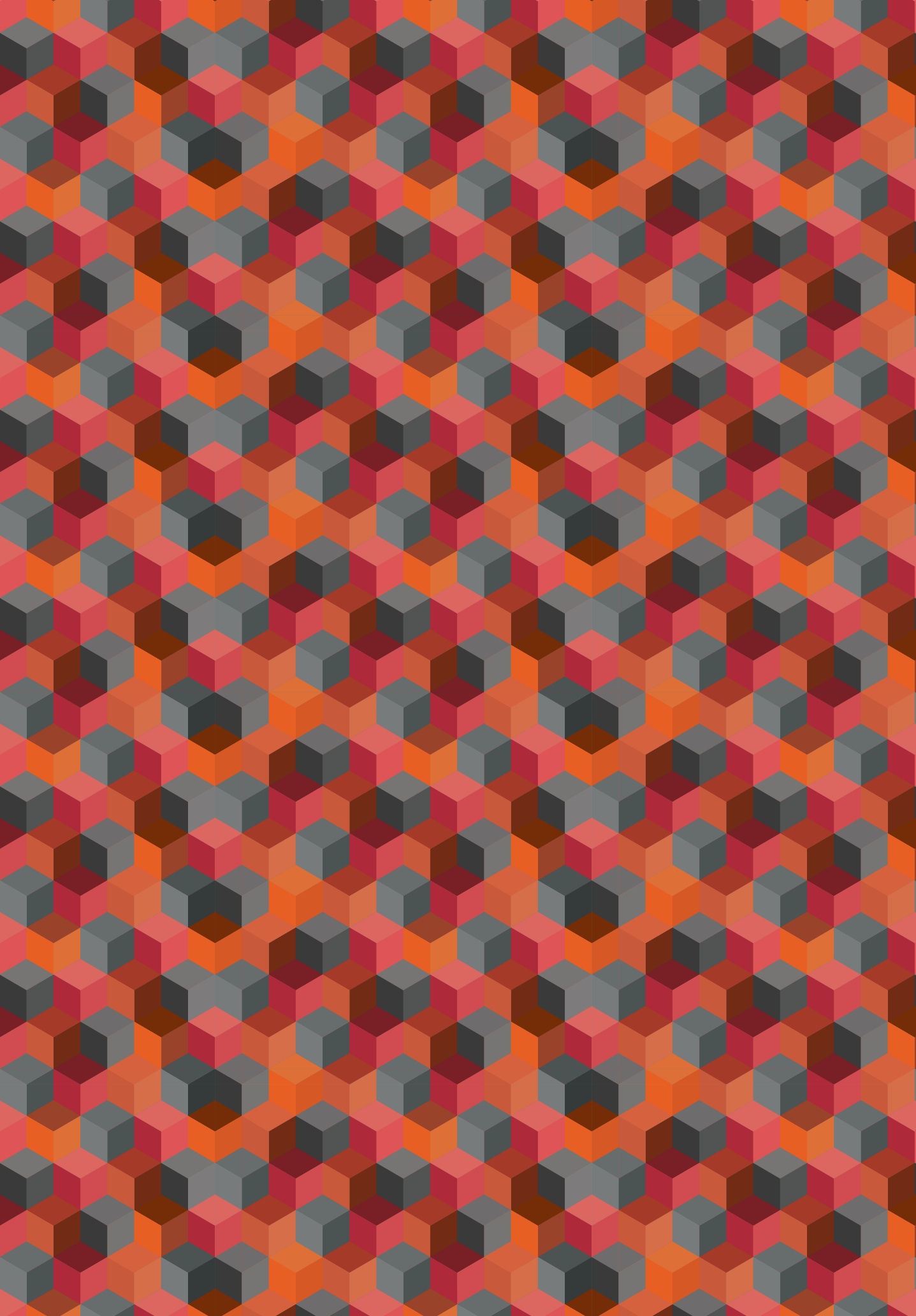


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Unibertsitatea



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Introduction

Materials Physics Center / Materialen Fisika Zentrua / Centro de Física de Materiales (CFM) is a joint center between the Spanish Scientific Research Council (CSIC) and the University of the Basque Country (UPV/EHU).

CFM was created in 1999 and holds its headquarters in Donostia – San Sebastián.

Since 2010, CFM occupies its own building in the Ibaeta Campus of UPV/EHU.

CFM is distinguished as a “Basque Excellence Research Center” by the Basque Government (BERC Program).

The CFM activity addresses several targets:

Generation of new knowledge based on research excellence

This is the primary goal of the Center. CFM carries on fundamental research on materials science, condensed matter physics, nanoscience, and related fields, at the highest international level, thanks to a balanced combination of theoretical and experimental efforts. The research lines that currently define the scientific activity of CFM and MPC are the following:

- ◆ Chemical Physics of Complex Materials
- ◆ Electronic Properties at the Nanoscale
- ◆ Photonics
- ◆ Polymers and Soft Matter

Training

One of the natural outputs of research excellence is that the training of young scientists contributes to further spread this excellence in the educational and economical environments. CFM is aware of the crucial role that education and training plays in the scientific and technological development of society. Being

a joint center between CSIC and UPV/EHU, CFM is a privileged agent to fulfill this goal. CFM is committed to design and participate in academic programs both at the undergraduate and graduate level. The official UPV/EHU program “Master in Nanoscience”, in whose organization CFM is involved, is a relevant example of this commitment.

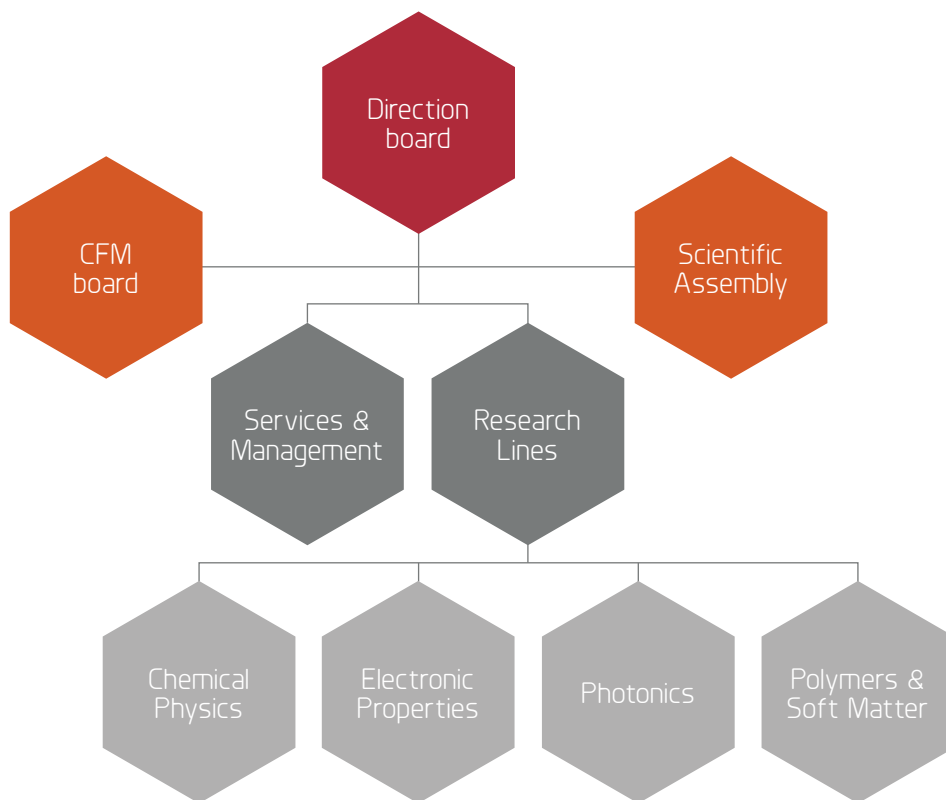
Transfer of knowledge

From a local perspective, CFM plays an important role in the network of scientific research centers emerging in San Sebastian or nearby. Being a basic research center but extremely well connected to other more applied centers, CFM should work as a catalyzer in the transfer of knowledge between institutions devoted to basic research and the wide network of technological centers and companies dedicated to Research and Development (R+D) in the Basque Country.

Science communication

Last, but not least, CFM pretends to be a dynamical actor in disseminating and popularizing science and the scientific activity through society.

Governance



Current Direction Board:

Director: Ricardo Díez Muiño

Deputy Director: Iñaki Juaristi Oliden

Secretary: Angel Alegria Loinaz

CFM Board:

Members of this board include the full direction board, the coordinators of each of the four research lines of the center, two representatives of the scientific personnel of the CFM, as well as one representative of the 'Services and Management' section.

CFM Scientific Assembly:

All scientific permanent staff of the CFM participate in the Scientific Assembly. The Assembly is thus made of UPV staff, CSIC staff, as well as Ikerbasque staff.



Human Resources



DIRECTION

Ricardo Diez Muiño, Director
Joseba Iñaki Juaristi Oliden, Deputy Director
Angel Alegria Loinaz, General Secretary

MANAGEMENT

Staff

Amaya Moral Arce, Manager, CSIC
Elixabete Mendizabal Ituarte, Executive Secretary, UPV/EHU
Jose Maria Ramos Fernández, Administrative, CSIC

Non-Permanent members

Maria Formoso Ferreira, Administrative, MPC
Francisco Lopez Gejo, Project Manager, MPC

COMPUTING SERVICES

Staff

Iñigo Aldazabal Mensa, Computer Center Manager, CSIC

Non-Permanent members

Garbiñe Egaña Cruz, IT Systems Technician, MPC

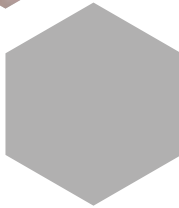
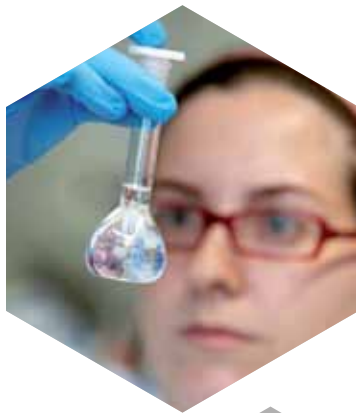
TECHNICAL SUPPORT

Staff

Silvia Arrese-Igor Irigoyen, Technician R+D+I, CSIC
Luis Botana Salgueiro, Technician R+D+I, CSIC

Non-Permanent members

Maria Isabel Asenjo Sanz, Technician, MPC
Emilio Varela, Technician, CSIC



Research line:

CHEMICAL PHYSICS OF COMPLEX MATERIALS

Staff

Maite Alducin Ochoa, Tenured Scientist, CSIC
Andrés Arnau Pino, University Professor, UPV/EHU
Ricardo Díez Muiño, Tenured Scientist, CSIC
J. Iñaki Juaristi Oliden, Associate Professor, UPV/EHU
Jorge Lobo Checa, Tenured Scientist, CSIC
Enrique Ortega Conejero, University Professor, UPV/EHU
Celia Rogero Blanco, Tenured Scientist, CSIC
Daniel Sánchez Portal, Research Scientist, CSIC
Frederik Michael Schiller, Tenured Scientist, CSIC
Ivo Souza, Ikerbasque Professor
Lucia Vitali, Ikerbasque Professor

Postdoctoral Researchers

Patrizia Borghetti, MPC
Martina Corso, Ikerbasque Fellow
Mads Engelund, CSIC
Dimas García de Oteyza, UPV/EHU EC
Maxim Ilin, CSIC JAE
Petr Koval, CSIC JAE
David Frederick Pickup, MPC
Laura Natalia Serkovic Loli, UPV/EHU
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PhD Students

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Alexander Correa Aristizabal, DIPC
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Giuseppe Foti UPV/EHU
Oihana Galparsoro Larraza, UPV/EHU
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Elizabeth Goiri Little, DIPC
Natalia Koval, CSIC Jae Predoc
Ivor Lončarić, MPC
Ana Magaña Vicandi, UPV/EHU FPI
Federico Marchesin, MPC
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Maider Ormaza Saezmiera, UPV/EHU

Research line:

ELECTRONIC PROPERTIES AT THE NANOSCALE

Staff

Andrés Ayuela Fernández, Research Scientist, CSIC
Aitor Bergara Jauregi, Associate Professor, UPV/EHU
F. Sebastian Bergeret Sbarbaro, Tenured Scientist, CSIC
Eugene V. Chulkov, University Professor, UPV/EHU
Pedro Miguel Echenique Landiribar, University Professor, UPV/EHU
José María Pitarke de la Torre, University Professor, UPV/EHU
Angel Rubio Secades, University Professor, UPV/EHU

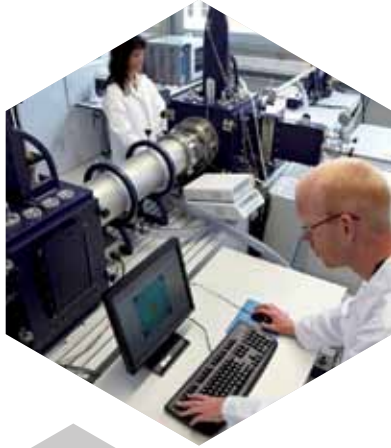
Postdoctoral Researchers

Vitaly Golovach, Ikerbasque Fellow
Jhon Wilfer González Salazar, MPC
Miguel Ángel Gosálvez, UPV/EHU Ramón y Cajal
Seymur Jahangirov, CSIC JAE
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Amilcare Iacomino, CSIC JAE
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PhD Students

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Juan Pablo Echeverry Enciso, DIPC
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Ainhoa Suárez Alcubilla, CSIC
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Sadique Vellarmarthodika Mohammed, GV-EJ
Jessica Walkenhorst, FPU





Research line:

PHOTONICS

Staff

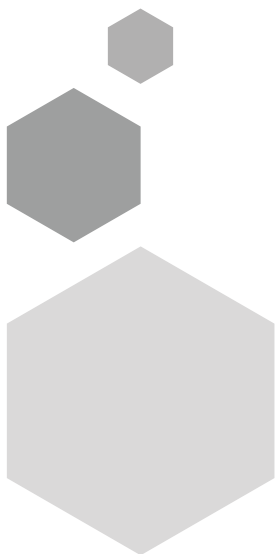
Fco. Javier Aizpurua Iriazabal, Research Scientist, CSIC
Rolindes Balda de la Cruz, University Professor, UPV/EHU
Joaquin Fernández Rodríguez, University Professor, UPV/EHU
Yury Rakovich, Scientist, Professor Ikerbasque
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PhD Students

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Mohamed Ameen Poyli, MPC
Mikolaj Schmidt, CSIC



Research line:

POLYMERS AND SOFT MATTER

Staff

Angel Alegría Loinaz, University Professor, UPV/EHU
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Silvina Cervený Murcia, Tenured Scientist, CSIC
Juan Colmenero de León, University Professor, UPV/EHU
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Guido Goracci, MPC
Yasmin Khairy, MICINN FPI
Mohammed Musthafa Kummali, UPV/EHU
Alejandro Latorre Sánchez, MPC
Gerardo Martinez Rogero, MPC
Manuel Monasterio, MPC
Irma Pérez Baena, CSIC Jae Predoc
Ana Belén Sánchez Sánchez, UPV/EHU
Zakaria Slimani, DIPC

OTHER POSITIONS

Staff

Isabel Telleria Echeverria, Associate Professor, UPV/EHU
Juan José del Val Altuna, Associate Professor, UPV/EHU

Infrastructure and Equipment



As of December 2013, the facilities installed at our Center are the following:

Ultra-low Temperature Scanning Tunneling Microscopy Lab

A combined AFM/STM instrument capable of scanning atomic forces and tunneling current simultaneously at 1 K.

High Resolution Angle Resolved Photoemission Lab

A combined ARPES/STM system with a double prep-chamber, which permits separate and joint ARPES/STM experiments. The ARPES chamber is an ultra-high resolution (0.1 degree, 5 meV) system, able of measuring solid samples down to 20 K.

Surface Chemistry and Magnetism Lab

Two separate STM/X Ray Photoemission (XPS) and STM/Magneto Optic Kerr Effect (MOKE) chambers for surface chemistry and surface magnetism experiments, respectively.

Nanophotonics Lab

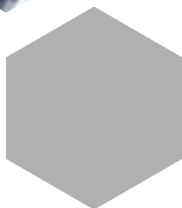
Scanning confocal time-resolved photoluminescence setup (Micro-Time200, PicoQuant) providing single molecule sensitivity and high temporal resolution. Range of application includes Fluorescence Lifetime Imaging (FLIM), Fluorescence Correlation Spectroscopy (FCS), Forster Resonance Energy Transfer (FRET), Fluorescence Lifetime Measurements, Fluorescence Anisotropy and Intensity Time Traces.

Spectroscopy Techniques

Spectroscopic equipment (Cary50, Varian) for measurement of energy transfer and conversion.

Laser Spectroscopy Lab

Continuous and time-resolved (with nano-pico excitation laser sources) spectroscopies with high spectral resolution in the UV-VIS-IR domains together with low temperature facilities (2K). Home made photoacoustic spectrometer.



Ultrafast Spectroscopy Lab

Tunable femtosecond sources (with regenerative amplification) in the IR domain with high speed detectors in the picosecond domain (Streak camera). Multiphoton microscope with time-resolved spectroscopic facilities.

Material Synthesis Lab

Crystal growth facilities by using home made Bridgman and Czochralski furnaces.

Dielectric Spectroscopy Lab

Different frequency and time-domain spectrometers covering more than 16th orders of magnitude in frequency/time.

Molecular Spectroscopy Techniques

Infrared Spectrometer FT-IR, Terahertz Spectrometer.

Microscopy Lab

Atomic Force Microscope (AFM), Optical/Confocal Microscope, Desktop Scanning Electron Microscope.

X-ray Lab

Small Angle X-Ray Scattering (SAXS) technique: Rigaku PSAXS-L, Wide Angle X-Ray Scattering (WAXS) with the same instrument.

Thermal Analysis Techniques

Differential Scanning Calorimetry (DSC), Pressure-Volume-Temperature (PVT), Thermogravimetric Analysis (TGA), Dilatometry (DIL).

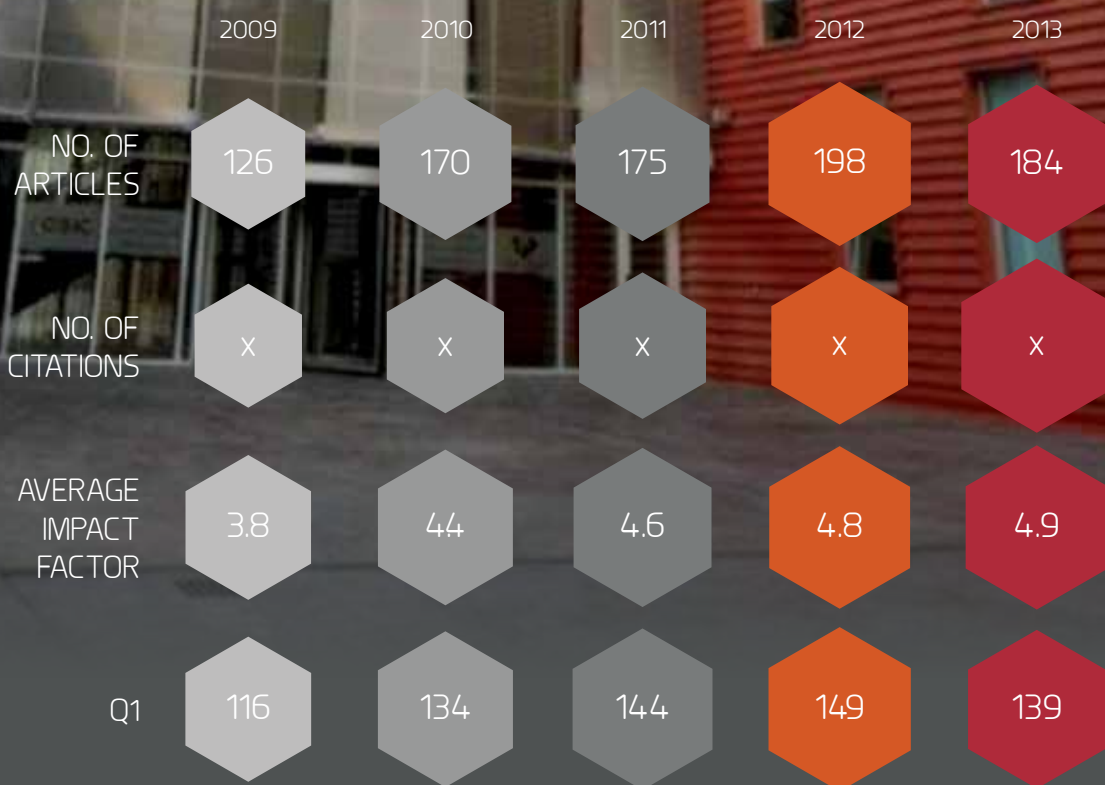
Chemistry Lab

Different techniques oriented to Polymer Synthesis and Click-Chemistry.

Computing Facilities for Ab initio Calculations and Other Simulation Methods

Several computing clusters at CFM. Several scientific codes for ab initio calculations (DFT based on plane waves and local orbitals, quantum chemistry, quantum Monte Carlo), as well as other computational and graphic packages. Several scientific codes for solving Maxwell equations, based on finite differences in time domain (e.g., Lumerical solutions), discrete dipole approximation (DDA), etc. Software for atomistic and coarse-grained MD-simulations.

Research output





Publications

1

“Michael” Nanocarriers Mimicking Transient-Binding Disordered Proteins

Sanchez-Sanchez A, Akbari S, Etxeberria A, Arbe A, Gasser U, Moreno AJ, Colmenero J, Pomposo JA.
ACS Macro Letters 2, 491 (2013)

2

Endowing single-chain polymer nanoparticles with enzyme-mimetic activity

Perez-Baena I, Barroso-Bujans F, Gasser U, Arbe A, Moreno AJ, Colmenero J, Pomposo JA.
ACS Macro Letters 2, 775 (2013)

3

Large Enhancement of Nonlinear Optical Response in a Hybrid Nanobiomaterial Consisting of Bacteriorhodopsin and Cadmium Telluride Quantum Dots

Rakovich A, Nabiev I, Sukhanova A, Lesnyak V, Gaponik N, Rakovich YP, Donegan JF.
ACS Nano 7, 2154 (2013)

4

Tunable Molecular Plasmons in Polycyclic Aromatic Hydrocarbons

Manjavacas A, Marchesin F, Thongrattanasiri S, Koval P, Nordlander P, Sánchez-Portal D, de Abajo FJG.
ACS Nano 7, 3635 (2013)

5

Tailored Formation of N-Doped Nanoarchitectures by Diffusion-Controlled on-Surface (Cyclo)-Dehydrogenation of Heteroaromatics

Pinardi AL, Otero-Irurueta G, Palacio I, Martinez JI, Sanchez-Sanchez C, Tello M, Rogero C, Cossaro A, Preobrajenski A, Gomez-Lor B, Jancarik A, Stara IG, Stary I, Lopez MF, Mendez J, Martin-Gago JA.
ACS Nano 7, 3676 (2013)

6

Tuning the band gap of graphene nanoribbons synthesized from molecular precursors

Chen YC, de Oteyza DG, Pedramrazi Z, Chen C, Fischer FR, Crommie MF.
ACS Nano 7, 6123 (2013)

7

Understanding Energy-Level Alignment in Donor-Acceptor/Metal Interfaces from Core-Level Shifts

El-Sayed A Borghetti P Goiri E Rogero C Floreano L Lovat G Mowbray DJ Cabellos JL Wakayama Y Rubio A Ortega JE de Oteyza DG.
ACS Nano 7, 6914 (2013)

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Octagonal Defects as the Source of Gap States in Graphene Semiconducting Structures

Pelc M, Jaskolski W, Ayuela A, Chico L.
Acta Physica Polonica A 124, 777 (2013)

9

Hydration and Dynamic State of Nanoconfined Polymer Layers Govern Toughness in Nacre-mimetic Nanocomposites

Verho T, Karesoja M, Das P, Martikainen L, Lund R, Alegria A, Walther A, Ikkala O.
Advanced Materials 25, 5055 (2013)

10

Enhancing the sensitivity of chemiresistor gas sensors based on pristine carbon nanotubes to detect low-ppb ammonia concentrations in the environment

Rigoni F, Tognolini S, Borghetti P, Drera G, Pagliara S, Goldoni A, Sangaletti L.
Analyst 24, 7392 (2013)

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Phase-tunable colossal magnetothermal resistance in ferromagnetic Josephson valves

Giazotto F, Bergeret FS.
Applied Physics Letters 102, 132603 (2013)

12

Quantum interference hybrid spin-current injector

Giazotto F, Bergeret FS.
Applied Physics Letters 102, 162406 (2013)

13

Efficient electron refrigeration using superconductor/spin-filter devices

Kawabata S, Ozaeta A, Vasenko AS, Hekking FWJ, Bergeret FS.
Applied Physics Letters 103, 032602 (2013)

14

Nanoscale texture development of C-S-H gel: A computational model for nucleation and growth

Gonzalez-Teresa R, Dolado JS, Ayuela A, Gimel JC.
Applied Physics Letters 103, 234105 (2013)

15

Thermal rectification of electrons in hybrid normal metal-superconductor nanojunctions

Giazotto F, Bergeret FS.
Applied Physics Letters 103, 242602 (2013)

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Bottom-up graphene nanoribbon field-effect transistors

Bennett PB, Pedramrazi Z, Madani A, Chen YC, de Oteyza DG, Chen C, Fischer FR, Crommie MF, Bokor J.
Applied Physics Letters 103, 253114 (2013)

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SiGe quantum dots for fast hole spin Rabi oscillations

Ares N, Katsaros G, Golovach VN, Zhang JJ, Prager A, Glazman LI, Schmidt OG, De Franceschi S.
Applied Physics Letters 103, 263113 (2013)

18

Electronic structure of SnSb₂Te₄ and PbSb₂Te₄ topological insulators

Menshchikova TV, Ereemeev SV, Chulkov EV.
Applied Surface Science 267, 1 (2013)

19

Bulk and surface electronic structure of SnBi₄Te₇ topological insulator

Vergniory MG, Menshchikova TV, Ereemeev SV, Chulkov EV.
Applied Surface Science 267, 146-149 (2013)

20

Influence of the Ge-Sb sublattice atomic composition on the topological electronic properties of Ge₂Sb₂Te₅

Silkin IV, Koroteev YM, Bihlmayer G, Chulkov EV.
Applied Surface Science 267, 169 (2013)

21

Stress-induced buried waveguides in the 0.8CaSiO₃-0.2Ca₃(PO₄)₂ eutectic glass doped with Nd³⁺ ions

Sola D, de Mendibil JM, de Aldana JRV, Lifante G, Balda R, de Aza AH, Pena P, Fernandez J.
Applied Surface Science 278, 289 (2013)

22

Effective interactions of knotted ring polymers

Narros A, Moreno AJ, Likos CN.
Biochemical Society Transactions 41, 630 (2013)

23

Suitability of amorphous TiO₂ nanoparticles as a photoelectrode in dye sensitized solar cells: A DFT-TDDFT study

Eithiraj RD, Geethalakshmi KR.
Chemical Physics Letters 585, 138 (2013)

24

Structure, Atomistic Simulations, and Phase Transition of Stoichiometric Yeelimite

Cuesta A, De la Torre AG, Losilla ER, Peterson VK, Rejmak P, Ayuela A, Frontera C, Aranda MAG.
Chemistry of Materials 25, 1680 (2013)

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The Isolation of Single MMX Chains from Solution: Unravelling the Assembly-Disassembly Process

Azani MR, Paz AP, Hermosa C, Givaja G, Gomez-Herrero J, Mas-Balleste R, Zamora F, Rubio A.
Chemistry-A European Journal 19, 15518 (2013)

26

Simulating Pump-Probe Photoelectron and Absorption Spectroscopy on the Attosecond Timescale with Time-Dependent Density Functional Theory

De Giovannini U, Brunetto G, Castro A, Walkenhorst J, Rubio A.
Chemphyschem 14, 1363 (2013)

27

Implementation and evaluation of the Level Set method: Towards efficient and accurate simulation of wet etching for microengineering applications

Montoliu C, Ferrando N, Gosalvez MA, Cerda J, Colom RJ.
Computer Physics Communications 184, 2299 (2013)

28

Model for the Formation of Helium Bubbles in Palladium

Alonso JA, and Ayuela A.
Croatia Chemica Acta 86, 425, (2013)

29

Néel Temperature of Antiferromagnets for Phase Transitions Driven by Spin-wave Interactions

Ayuela A, Klein DJ and March NH.
Croatia Chemica Acta 86, 463, (2013)

30

Low temperature red luminescence of a fluorinated Mn-doped zinc selenite

Orive J, Balda R, Fernandez J, Lezama L, Arriortua MI.
Dalton Transactions 42, 12481 (2013)

31

One-step wet chemical deposition of NiO from the electrochemical reduction of nitrates in ionic liquid based electrolytes

Azaceta E, Tuyen NT, Pickup DF, Rogero C, Ortega JE, Miguel O, Grande HJ, Tena- Zaera R.
Electrochimica Acta 96, 261 (2013)

32

Carbon nanotubes as heat dissipaters in microelectronics

Paz AP, Garcia-Lastra JM, Markussen T, Thygesen KS, Rubio A.
European Physical Journal B 86, 234 (2013)

33

Efficient Step-Mediated Intercalation of Silver Atoms Deposited on the Bi₂Se₃ Surface

Otrokov MM, Borisova SD, Chis V, Vergniory MG, Ereemeev SV, Kuznetsov VM, Chulkov EV.
JETP Letters 96, 714 (2013)

34

New topological surface state in layered topological insulators: Unoccupied Dirac cone

Eremeev SV, Silkin IV, Menshchikova TV, Protogenov AP, Chulkov.
JETP Letters 96, 780 (2013)

35

Interface-induced states at the boundary between a 3D topological insulator and a normal insulator

Men'shov VN, Tugushev VV, Chulkov EV.
JETP Letters 97, 258 (2013)

36

Many-body effects on the width of the band gap in Bi₂Te₂X (X = Te, Se, S) topological insulators

Rusinov IP, Nechaev IA, Chulkov EV.
JETP Letters 98, 397 (2013)

37

Design of solar cell materials via soft X-ray spectroscopy

Himpfel FJ, Cook PL, de la Torre G, Garcia-Lastra JM, Gonzalez-Moreno R, Guo JH, Hamers RJ, Kronawitter CX, Johnson PS, Ortega JE, Pickup D, Ragoussi ME, Rogero C, Rubio A, Ruther RE, Vayssieres L, Yang W, Zegkinoglou I.
Journal of Electron Spectroscopy and Related Phenomena 190, 2 (2013)

38

Pressure induced phase transitions in TiH₂

Gao GY, Bergara A, Liu GT, Ma YM.
Journal of Applied Physics 113, 103512 (2013)

39

Correlation effects in the optical spectra of porphyrin oligomer chains: Exciton confinement and length dependence

Hogan C, Palumbo M, Gierschner J, Rubio A.
Journal of Chemical Physics 138, 024312 (2013)

40

Electronic structure of Fe- vs. Ru-based dye molecules

Johnson PS, Cook PL, Zegkinoglou I, Garcia-Lastra JM, Rubio A, Ruther RE, Hamers RJ, Himpfel FJ.
Journal of Chemical Physics 138, 044709 (2013)

41

On the interactions between poly(ethylene oxide) and graphite oxide: A comparative study by different computational methods

Garcia-Yoldi I, Alvarez F, Colmenero J.
Journal of Chemical Physics 138, 094308 (2013)

42

“Comment on “Unified explanation of the anomalous dynamic properties of highly asymmetric polymer blends”” [J. Chem. Phys. 138, 054903 (2013)]”

Colmenero J.

Journal of Chemical Physics 138, 197101 (2013)

43

Modeling the collective relaxation time of glass-forming polymers at intermediate length scales: Application to polyisobutylene

Colmenero J, Alvarez F, Khairy Y, Arbe A.

Journal of Chemical Physics 139, 044906 (2013)

44

Cause of the fragile-to-strong transition observed in water confined in C-S-H gel

Monasterio M, Jansson H, Gaitero JJ, Dolado JS, Cervený S.

Journal of Chemical Physics 139, 164714 (2013)

45

Theoretical study of influencing factors on the dispersion of bulk band-gap edges and the surface states in topological insulators Bi₂Te₃ and Bi₂Se₃

Rusinov IP, Nechaev IA, Chulkov EV.

Journal of Experimental and Theoretical Physics 116, 1006 (2013)

46

Near-infrared emission and upconversion in Er³⁺-doped TeO₂-ZnO-ZnF₂ glasses

Miguel A, Morea R, Gonzalo J, Arriandiaga MA, Fernandez J, Balda R.

Journal of Luminescence 140, 38 (2013)

47

Correlation Between Segmental Dynamics, Glass Transition, and Lithium Ion Conduction in Poly(Methyl Methacrylate) /Ionic Liquid Mixture

Jeddi K, Qazvini NT, Cangialosi D, Chen P.

Journal of Macromolecular Science Part B-Physycs 52, 590 (2013)

48

Atomic and electronic properties of quasi-one-dimensional MoS₂ nanowires

Seivane LF, Barron H, Botti S, Marques MAL, Rubio A, Lopez-Lozano X.

Journal of Materials Research 28, 240 (2013)

49

Explicit form of Pauli potential for direct derivation of pair density from a two-particle differential equation for the quintet state of four electrons with harmonic interparticle interactions

Akbari A, Amovilli C, March NH, Rubio A.

Journal of Mathematical Chemistry 51, 1462 (2013)

50

A proposed family of variationally correlated first-order density matrices for spinpolarized three-electron model atoms

Akbari A, March NH, Rubio A.

Journal of Mathematical Chemistry 51, 763 (2013)

51

Spectroscopy and energy transfer in Nd³⁺/Yb³⁺ codoped chalcogenide glasses

Miguel A, Fan B, Balda R, Zhang X, Fernandez J, Adam JL.

Journal of Non-crystalline Solids 377, 110 (2013)

52

Scattering of Nitrogen Atoms off Ag(111) Surfaces: A Theoretical Study

Martin-Gondre L, Bocan GA, Blanco-Rey M, Alducin M, Juaristi JJ, Muino RD.

Journal of Physical Chemistry C 117, 9779 (2013)

53

Spectroscopy of Donor- π -Acceptor Porphyrins for Dye-Sensitized Solar Cells

Zegkinoglou I, Ragoussi ME, Pemmaraju CD, Johnson PS, Pickup DF, Ortega JE, Prendergast D, de la Torre G, Himpfel FJ.

Journal of Physical Chemistry C 117, 13357 (2013)

54

Low-Loss Electric and Magnetic Field-Enhanced Spectroscopy with Subwavelength Silicon Dimers

Albella P, Poyli MA, Schmidt MK, Maier SA, Moreno F, Saenz JJ, Aizpurua J.

Journal of Physical Chemistry C 117, 13573 (2013)

55

Strong Enhancement of Circular Dichroism in a Hybrid Material Consisting of JAggregates and Silver Nanoparticles

Melnikau D, Savateeva D, Gun'ko YK, Rakovich YP.

Journal of Physical Chemistry C 117, 13708 (2013)

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Large spin splitting of metallic surface-state bands at adsorbate-modified gold/silicon surfaces

Bondarenko LV, Gruznev DV, Yakovlev AA, Tupchaya AY, Usachov D, Vilkov O, Fedorov A, Vyalikh DV, Ereemeev SV, Chulkov EV, Zotov AV, Saranin AA.
Scientific Reports 3, 1826 (2013)

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Efficient Gate-tunable light-emitting device made of defective boron nitride nanotubes: from ultraviolet to the visible

Attaccalite C, Wirtz L, Marini A, Rubio A.
Scientific Reports 3, 2698 (2013)

178

Octagonal defects at carbon nanotube junctions

Jaskolski W, Pelc M, Chico L, Ayuela A.
Scientific World Journal 2013, 658292 (2013)

179

Confinement of poly(ethylene oxide) in the nanometer-scale pores of resins and carbon nanoparticles

Barroso-Bujans F, Palomino P, Cerveny S, Fernandez-Alonso F, Rudic S, Alegria A, Colmenero J, Enciso E.
Soft Matter 9, 10960 (2013)

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Fluids of semiflexible ring polymers: effective potentials and clustering

Bernabei M, Bacova P, Moreno AJ, Narros A, Likos CN.
Soft Matter 9, 1287 (2013)

181

Physical aging in polymers and polymer nanocomposites: recent results and open questions

Cangialosi D, Boucher VM, Alegria A, Colmenero J.
Soft Matter 9, 8619 (2013)

182

Exploring large O 1s and N 1s core level shifts due to intermolecular hydrogen bond formation in organic molecules

Garcia-Gil S, Arnau A, Garcia-Lekue A.
Surface Science 613, 102 (2013)

183

Glass transition and segmental dynamics in thin supported polystyrene films: The role of molecular weight and annealing

Yin H, Cangialosi D, Schonhals A.

Thermochimica Acta 566, 186 (2013)

184

Ready, Set and no Action: A Static Perspective on Potential Energy Surfaces commonly used in Gas-Surface Dynamics

Bukas VJ, Meyer J, Alducin M, Reuter K.

Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics 227, 1523 (2013)

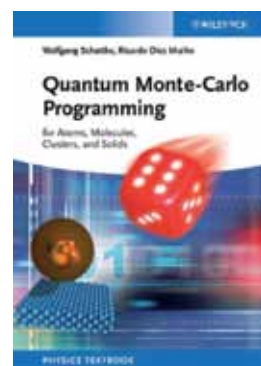
BOOKS AND BOOK CHAPTERS

Books

Quantum Monte-Carlo Programming for Atoms, Molecules, Clusters, and Solids

Wolfgang Schattke and R. Díez Muiño

(Wiley-VCH, Berlin 2013), ISBN 978-3-527-40851-1.



Dynamics of gas/surface interactions: Atomic-level understanding of scattering processes at surfaces

Edited by R. Díez Muiño and H. F. Busnengo

'Springer Series of Surface Sciences' vol. 50 (Springer, Berlin 2013), ISBN 978-3-642-32954-8.

Book chapters

Energy dissipation channels in reactive and non-reactive scattering at surfaces

M. Alducin, R. Díez Muiño, and J. I. Juaristi

chapter 15 in 'Dynamics of Gas-Surface Interactions'

Ed. by R. Díez Muiño and H. F. Busnengo

(Springer, 2013)

Optical antennas for field-enhanced spectroscopy

J. Aizpurua and R. Esteban

chapter 5 Optical Antennas (Cap.5): 64-79

(Cambridge University Press, 2013)

Highlights


Among all scientific articles written by CFM scientists in 2013, let us list below the number of them published in high impact-factor journals:

	Nº ART.	IMPACT FACTOR
Nature	1	38,597
Science	1	31,027
Advanced Materials	1	14,829
Nano Letters	5	13,025
ACS Nano	5	12,062
JACS	2	10,677
Nature Communications	1	10,015
Chemistry of Materials	1	8,238
Physical Review Letters	15	7,943

Further research activity



- ◆ CFM scientists have delivered 60 invited and plenary talks in the year 2013 to spread their research results, most of them in specialized international conferences and workshops.
- ◆ CFM scientists have contributed with 65 oral talks in the year 2013 to spread their research results, most of them in specialized international conferences and workshops. Young scientists were responsible for a significant amount of these oral contributions.
- ◆ CFM scientists have organized 2 workshops in the year 2013. These meetings have been held in close cooperation with Donostia International Physics Center (DIPC), which proves the excellent results brought by the synergy between both institutions. The list follows:
 - **BRW – 30th Brand Rithie Workshop** Octubre 1-4, 2013. CFM, Material Physics Center, Donostia - San Sebastián - DIPC and Euskampus
 - **Baskrete – Industry open days** Mayo 28-29, 2013. Donostia - San Sebastián - CEI Euskampus - EHU/UPV - DIPC -Tecnalia - CFM - CIC nanoGUNE
- ◆ CFM organizes a program of informal seminars in which local researchers, not only from CFM but also from other local research centers (UPV/EHU, CICs, BERCs) give a broad overview of their research activity. This program has shown to be a useful tool to boost collaboration among different agents of the local scientific tissue.

- 
- ◆ Los CFM scientists keep active collaborations with researchers from other worldwide institutions. We list below some of the researchers with which at least one joint article has been published in 2013 as a result of the collaboration:

Chemical Physics of complex Materials

- Yutaka Wakayama (Tsukuba, Japan)
- Dietrich Foerster (Université Bordeaux I, France)
- Franz Himpsel (Univ.of Madison Wisconsin, USA)
- David Vanderbilt (Rutgers University, USA)
- Geert-Jan Kroes (Leiden University, Netherlands)

Photonics

- Peter Nordlander (Rice University, Houston, USA)
- Annemarie Pucci (Univ. of Heidelberg, Germany)
- Garnett W. Bryant (NIST, Washington, USA)
- Mikael Käll (University of Chalmers, Sweden)
- Jeremy Baumberg (University of Cambridge, UK)

Polymers and Soft Matter

- D. Richter (JCNS Jülich, Germany)
- B. Frick (ILL Grenoble, France)
- R. P. Quirk (University of Akron, USA)
- R. Arinero (Université Montpellier2, France)
- P. Tordjeman (CNRS Toulouse, France)

Electronic Properties in the Nanoscale

- Ferenc Krausz (MPI Garching, Germany)
- J. P. Toennies (University of Göttingen, Germany)
- Tadaaki Nagao (MANA, Japan)
- Marvin Cohen / Steven Louie (UC Berkeley, USA)
- Klaus Kern (MPI Stuttgart, Germany)

Research funding



Grant Agreement 267374, 7PM-IDEAS

Dynamical processes in open quantum systems: pushing the frontiers of theoretical spectroscopy.

PI: A. Rubio

FIS2010-19609-C02-01

Dinámica electrónica, transporte, plasmonica y microscopia electrónica.

PI: A. Arnau

FIS2010-19609-C02-02

Propiedades electrónicas y reactividad de sistemas complejos.

PI: R. Díez Muiño

FIS2010-21282-C02-01

Estudio de la dinámica de sistemas cuánticos complejos: desde desarrollos teóricos fundamentales a aplicaciones energéticas (captura, almacenamiento, transmisión).

PI: A. Rubio

MAT2010-21156-C03-01

Desarrollo y análisis de agregados nanoestructurados moleculares y magnéticos para aplicaciones en células solares y de almacenamiento de datos

PI: E. Ortega

MAT2010-21156-C03-03

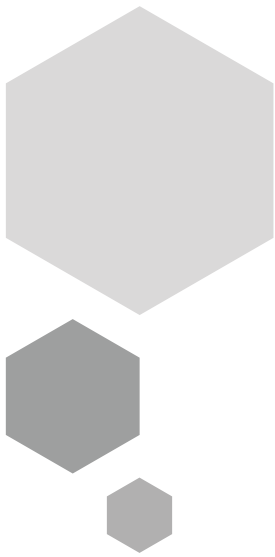
Desarrollo y análisis de agregados nanoestructurados moleculares y magnéticos para aplicaciones en células solares y de almacenamiento de datos.

PI: F. Schiller

FIS2011-27968

Estudio comparativo de la dinámica espectral y temporal de láseres aleatorios bajo excitación a uno y dos fotones en un mismo medio dispersor.

PI: J. Fernández



FIS2011-28851-C02-02

Propiedades de transporte electrónico en nanoestructuras híbridas: superconductores, ferro magnetos y metales normales.

PI: F. S. Bergeret

PITN-GA-2012-316633 POCAONTAS

Polymer - Carbon Nanotubes Active Systems for Photovoltaics POCAONTAS

PI: A. Rubio

MAT2010-21156-C03-01

Espectroscopia túnel y fotoemisión de moléculas, agregados y estructuras autoensambladas en superficies sólidas.

PI: E. Ortega

SAI11/237

Propiedades electrónicas y estructurales de superficies limpias o funcionalizadas de aislantes topológicos.

PI: L. Vitali

SAI12/202

Propiedades magnéticas y electrónicas de aleaciones bi-dimensionales de gadolinio y de sus enlaces con moléculas orgánicas.

PI: L. Vitali

GIC12/109

Caracterización topográfica y espectroscópica de nano-estructuras sobre superficies con microscopio de efecto túnel a la temperatura de 1 grado kelvin.

PI: L. Vitali

NMP3-SL-2012-280879

Time dynamics and Control in nanoStructures for magnetic recording and energy applications”

CRONOS

PI: A. Rubio

PLASMON

Enhancement effects in plasmonic nanocavities formed at metal nanowire junctions

PI: Y. Rakovich

PITN-GA-2008-214627

DYNACOP: DYNamics of Architecturally COMplex Polymers

PI: J. Colmenero

IT654-13

Grupos de Investigación Consolidados / de Alto Rendimiento: “Polímeros y materiales no cristalinos”

PI: J. Colmenero

IT578-13

Grupos de Investigación Consolidados / de Alto Rendimiento: “

PI: A. Rubio

IT621-13

Grupos de Investigación Consolidados / de Alto Rendimiento: “Laboratorio de Nanofísica”

PI: E. Ortega

IT756-13

Grupos de Investigación Consolidados / de Alto Rendimiento:

PI: A. Arnau

FP7-ICT-2013-10 610446

PAMS - Planar Atomic and Molecular Scale devices

PI: D. Sánchez

IT

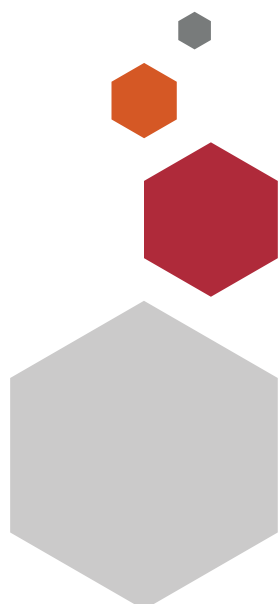
Grupos de Investigación Consolidados / de Alto Rendimiento:

PI: J. Fernández

MAT2012-33720

Efectos magnetoeléctricos estáticos y ópticos en cristales

PI: Ivo Souza



Training



CFM is part of University of the Basque Country UPV/EHU and thus shares its mission on higher education, in particular at post-graduate level. CFM is one of the very few centers of the Basque Country in which a balanced body of University teachers/researchers and purely research staff (CSIC and Ikerbasque researchers) coexist and interact on a regular basis. The standard PhD education for a young student at CFM goes through two stages:

- ◆ Master's in Nanoscience is an official program of UPV/EHU (held at CFM quarters) and coorganized by the CFM itself. The goal of the Master in Nanoscience is to provide the student with the basic concepts and the most commonly used working tools in the field of Nanoscience, including the use and interpretation of the results of the experimental techniques that are specific of the Nanotechnology research laboratories, topics related to the nanomaterials and their applications, and a general knowledge on the research activity at the international level in the field of Nanoscience. In addition, during his/her Master's thesis work, the student will choose to develop either the skills that are necessary in the applied and technology-oriented research work pursued in Technological Centers, or those necessary in the basic/oriented research that is carried out in academic research groups. The students will be also able to start developing the research work that may allow them to obtain the PhD degree.
- ◆ Physics of Nanostructures and Advanced Materials is a Ph.D. program of the University of the Basque Country (UPV/EHU) which has been recognized by the Spanish Ministry of Education as a highly-qualified Ph.D. program (Mención hacia la excelencia MEE2011-0591). After completing a master program (usually the Master's in Nanoscience program, although other similar degrees are accepted as well), the PhD student joins one of the research groups at the Center and is trained to develop his/her own research work. The PhD Committee of Graduate Studies looks after the PhD student training on an individual basis. The list of PhD thesis works successfully defended at CFM in 2013 follows:

PhD Theses

1.

"Structure-Dependent Electronic Properties in Donor-Acceptor Assemblies on Metal Surfaces".

Afaf El-Sayed Abd El-Mottaleb, UPV/EHU

Supervisor: Enrique Ortega

Date: February 13 2013

2.

“Reactivity and dynamics of N² and O² molecules on different metal surfaces”.

Itziar Goikoetxea Martinez, UPV/EHU.

Supervisor: Iñaki Juaristi and Maite Alducin

Date: February 21 2013

3.

“Bosons and Fermions in Mixed-dimensional Optical Lattices: Phase equilibria and Quantum Phase Transitions”.

Eneko Malatsetxebarria Elizegi, UPV/EHU.

Supervisor: Miguel Ángel Cazalilla

Date: May 10 2013

4.

“Rare earth/Noble metal surface alloys”

Maidier Ormaza Saezmiera, UPV/EHU

Supervisor: Enrique Ortega

Date: June 11 2013

5.

“Static and time-dependent density functionals for non-linear processes”

Johanna Fuks, UPV/EHU

Supervisor: Angel Rubio

Date: June 2013

6.

“Slow Dynamics in Nanostructured Phases of Diblock, Gradient and Random Copolymers: A Computational Investigation”

Mohammed Zakaria Slimani, UPV/EHU

Supervisor: Ángel Moreno

Date: July 01 2013

7.

“Applications of maximally localized Wannier functions: spin-flip excitations, plasmon dispersion and tight binding models for optical lattices”

Julen Ibáñez Azpiroz, UPV/EHU

Supervisor: Aitor Bergara

Date: September 13 2013

8.

“Structure and Dynamics of Polyisobutylene. A Molecular Dynamics Simulations Study”

Yasmin Khairy Abd El-fatah, UPV/EHU

Supervisor: Fernando Alvarez and Arantxa Arbe

Date: September 27 2013

9.

“Theoretical Description of the Optical Properties of Nanostructures Within Time Dependent Density Functional Theory”

Leonardo Andrés Espinosa Leal, UPV/EHU

Supervisor: Ángel Rubio

Date: October 22 2013

10.

“On the Dielectric Properties of Polymers at Nanometric Scale by AFM Microscopy”

Mohammed Musthafa Kummali, UPV/EHU

Supervisor: Ángel Alegría and Gustavo Ariel Schwartz

Date: December 2 2013

Undergraduate Courses

In addition to that, staff at CFM deliver undergraduate courses in 4 Faculties and University Schools. More than 1200 hours of teaching spread over 6 undergraduate degrees plus 3 Master degrees.

PhD students seminars

Since 2013, a series of seminars delivered by PhD students is organized at CFM. Approximately every two weeks, from September to June, two PhD students present updated results of their thesis 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. Ikerbasque Professor Lucia Vitali and UPV/EHU Professor Nerea Zabala are the coordinators of this activity.

Outreach

- ◆ Science Week: Every year 2 stands aimed at explaining the activities of CFM are installed at the UPV/EHU Science Week in Donostia-San Sebastian in a joint initiative with CIC nanoGUNE and DIPC.
- ◆ CFM is developing a broad program of activities aimed at bringing the excitement of science to young people. Among these activities, particular effort is devoted to secondary-level and high-school students, with an overall goal of increasing student and teacher enthusiasm for scientific research. Since September 2013 and every two weeks, several schools have visited CFM facilities, again sharing efforts with DIPC:

	GRUPO	Nº ESTUDIANTES
Larramendi ikastetxea	4º ESO	32
Presentación de María ikastetxetik	4º ESO	25
IES Leizaran de AndoainNano	1º y 2º Bachiller	30
IPINTZA Bergarako Institutua	1º Bachiller	13
Beasain BHI	2º Bachiller	28
Usandizaga Institutua	2º Bachiller	41
Urretxu Zumarraga Ikastola	2º Bachiller	29

The CFM organizing committee for these visits is made of Jorge Lobo, Celia Rogero, and Daniele Cangialosi.



Knowledge Transfer and Innovation

While focused in fundamental research, CFM is committed to maximize the return over society and the economical tissue, offer new career routes to its students and young researchers and promote the transfer of technology towards industrial activities.

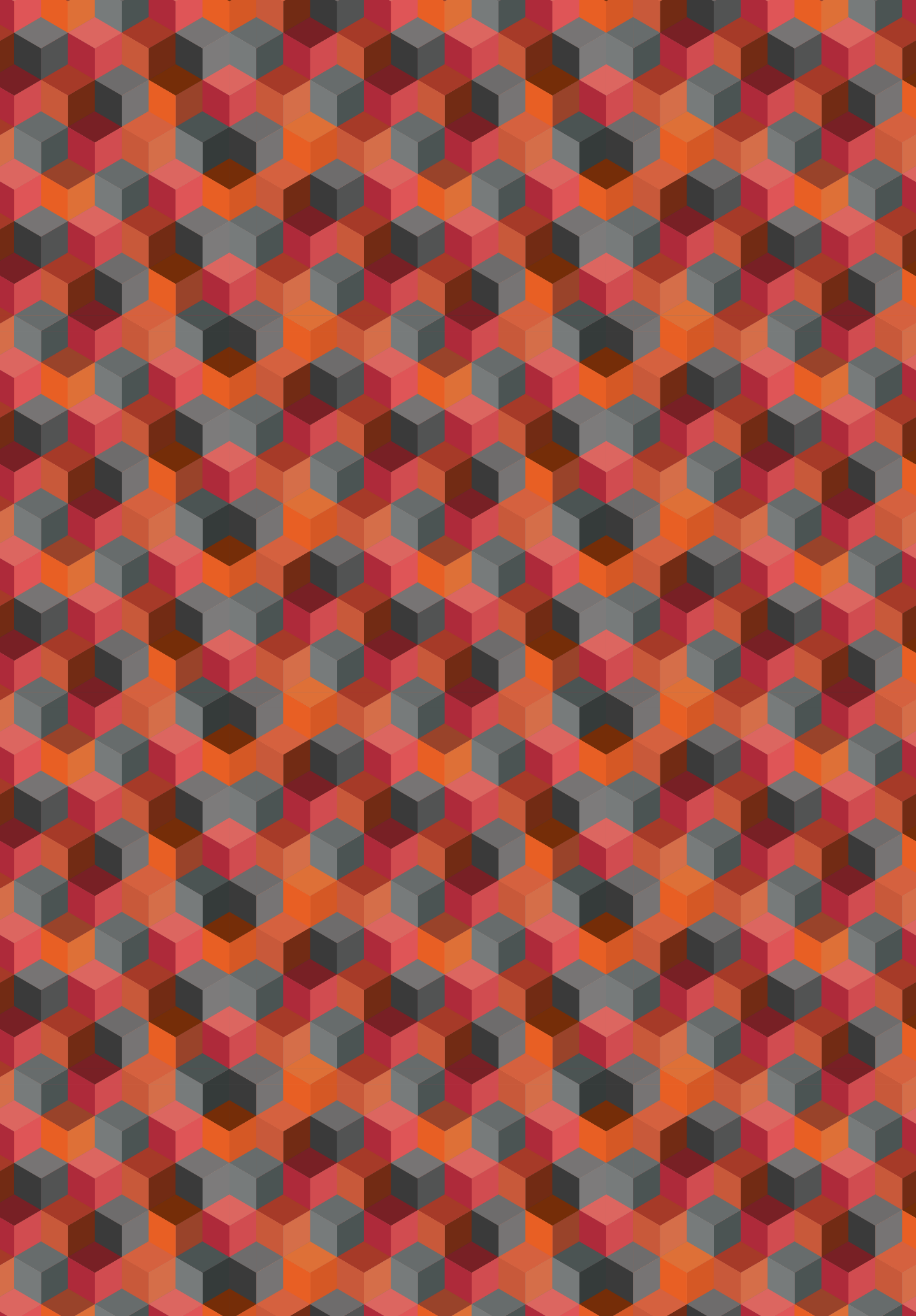
The spin-off program is a cornerstone for the achievement of these objectives. Through this program, CFM actively supports the development of entrepreneurial projects based in know-how and technologies developed within the center.

Special emphasis is applied in exploring innovative business models suitable for making economically viable the exploitation of state-of-the-art technologies. This stage is developed in collaboration with BIC Berrilan, through its Txekintek/Ekintzaile program.

There are currently three ongoing new enterprising projects:

- ◆ BIHURCRYSTAL S.L. Focused in the development of scientific equipment for vacuum and ultra-high vacuum applications. The aim is to exploit the rather large know-how accumulated by CFM research groups in this area, and take advantage of the unique advanced manufacturing capabilities of Gipuzkoa's industrial network. The company is already formally established and has started commercialization of its first products.
- ◆ GAINA SCA. Offers advanced engineering services for optimization of industrial processes and development of new products integrating new materials. These services rely heavily in the use of the start-of-the-art experimental techniques and infrastructure of the center.
- ◆ MORPHOKINETICS. Develops physical models and software for optimization of processes used for growing crystalline and bi-dimensional materials, such as graphene. The project has put together a multidisciplinary team formed by different groups of the UPV/EHU with backgrounds in Materials Science, Physics and Computer Science, who explore together innovative techniques for achieving accurate, computing efficient software.

CFM knowledge and technology is also made available to existing industries and companies directly. Several groups at CFM maintain collaborations with industries in different regions and across Europe for developing new products and processes. The center actively collaborates with the Technology Transfer Units of both CSIC and UPV/EHU for easing and speeding up the process of licensing of know-how and technology. CFM also provides Analysis Services, where industrial clients can request measurements using any of the state-of-the-art infrastructures available at CFM at affordable cost.





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