ACTIVITY REPORT 2014

Centro de Física de Materiales
Materials Physics Center

Materialen Fisika Zentroa

GOBIERNO DE ESPAÑA · MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD · CSIC

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Universidad del País Vasco · Euskal Herriko Unibertsitatea

CFM
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Euskal Herriko Unibertsitatea

Summary

Introduction

Centro de Física de Materiales (CFM) is a research center focused in Materials Science. Born in 1999 as a joint initiative between Consejo Superior de Investigaciones Científicas (CSIC) and Universidad del Pais Vasco – Euskal Herriko Unibertsitatea (UPV-EHU), the long term goal of CFM is to push forward the frontiers of knowledge in our areas of expertise, by putting together stable teams with a record of excellence in scientific research.

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.

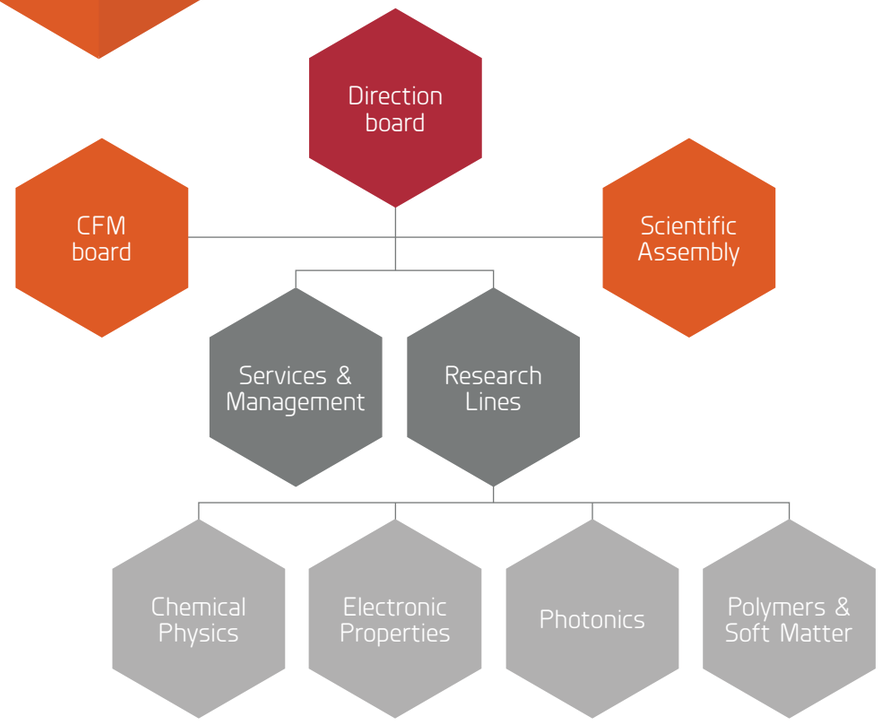
Transfer of knowledge

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 Alegría 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 in 2014

DIRECTION BOARD

Ricardo Díez Muiño, Director
Joseba Iñaki Juaristi Oliden, Deputy Director
Angel Alegría Loinaz, General Secretary

MANAGEMENT

Moral Arce, Amaia, Manager, CSIC
Mendizabal Ituarte, Elisabete, Executive Secretary, UPV/EHU (until September 2014)
Jose Maria Ramos Fernández, Administrative, CSIC
Jasone Ugarte Garcia de Andoin, Executive Secretary, UPV/EHU (since November 2014)
María Formoso Ferreiro, Administrative
Francisco López Gejo, Project Manager

COMPUTING SERVICES

Iñigo Aldazabal Mensa, Computer Center Manager, CSIC
Garbiñe Egaña Cruz, IT Systems Technician

TECHNICAL SUPPORT

Amaia Iturrospe Ibarra, Tecnician
Silvia Arrese-Igor Irigoyen, Technician R+D+I, CSIC
Luis Botana Salgueiro, Technician R+D+I, CSIC
Maria Isabel Asenjo Sanz, Technician
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

Ikerbasque Fellow

Martina Corso
Fernando Delgado

Postdoctoral Researchers

Patrizia Borghetti
Mads Engelund
Dimas García de Oteiza
Rubén González Moreno
Daniel Gosálbez
Maxim Ilin
Luis Alejandro Miccio
Thomas Olsen

PhD Students

Mikel Abadía Gutiérrez
Alexander Correa Aristizabal
Giuseppe Foti
Oihana Galparsoro Larraza
Elizabeth Goiri Little
Natalia Koval
Ivor Lončarić
Ana Magaña Vicandi
Federico Marchesin
Ahmed Mohamed Abdel Azim Nosir
Marc Barbry
Ignacio Piquero Zulaica
Iker Gallardo Arrieta
Moritz Mueller

Research line:

ELECTRONIC PROPERTIES AT THE NANOSCALE

Staff

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

Ikerbasque Fellow and RyC

Vitaly Golovach
Miguel Ángel Gosalvez

Postdoctoral Researchers

Jhon Wilfer González Salazar
Seymur Jahangirov
Elham Khosravi
Francois Xabier Konschelle
Daniel Rohr

PhD Students

Tomás Alonso Lanza
Miguel Borinaga Treviño
Asier Ozaeta Rodríguez
Ainhoa Suárez Alcubilla
Jessica Walkenhorst

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, Ikerbasque Professor
Alberto Rivacoba Ochoa, University Professor, UPV/EHU
Nerea Zabala Unzalu, Associate Professor, UPV/EHU

Postdoctoral Researchers

Sara García Revilla
Dzimitry Melnikau
Olalla Pérez Gonzalez
Diana Savateeva
Christos Tserkezis
Yao Zhang

PhD Students

Garikoitz Aguirregabiria Achutegi
Tomás Neuman
Mohamed Ameen Poyli
Mikolaj Schmidt

Research line:

POLYMERS AND SOFT MATTER

Staff

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

Postdoctoral Researchers

Fabienne Barroso Bujans
Ewa Golas
Federica Loverso
Luciana Saiz

PhD Students

Petra Bacova
Maria Luisa Barceló
Guido Goracci
Mohammed Musthafa Kummali
Alejandro Latorre Sánchez
Gerardo Martínez Rogero
Manuel Monasterio Jaqueti
Irma Pérez Baena
Ana Belén Sánchez Sánchez
Natalia Gutiérrez Pérez de Eulate
Izaskun Combarros Palacios
Marina González Burgos

OTHER POSITIONS

Staff

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

Research output 2014

NO. OF ARTICLES (ISI WoS)	170
NO. OF CITATIONS	7.121
AVERAGE IMPACT FACTOR	4.7

Among all scientific articles written by CFM scientists in 2014, let us list below the number of them published in high impact-factor journals:

JOURNAL	Nº ARTICLES	IMPACT FACTOR
Science	1	31,477
Accounts Of Chemical Research	1	24,348
Nano Letters	4	12,940
ACS Nano	3	12,033
J. Photochemistry and Photobiology C	1	11,625
Angewandte Chemie - International Edition	1	11,444
Journal of the American Chemical Society	1	11,336
Nature Communications	5	10,742
Laser & Photonics Reviews	1	9,313
Physical Review Letters	13	7,728
Small	1	7,514

Publication list

1

Spectroscopy of nitrophenolates in Vacuo: Effect of spacer, configuration, and microsolvation on the charge-transfer excitation energy

Nielsen, S.B.; Nielsen, M.B.; Rubio, A.

Accounts of Chemical Research 47, 1417 (2014)

2

Chain dynamics on crossing the glass transition: Nonequilibrium effects and recovery of the temperature dependence of the structural relaxation

Arrese-Igor, S.; Alegría, A.; Colmenero, J.

ACS MACRO LETTERS 3,1215 (2014)

3

Cluster glasses of semiflexible ring polymers

Slimani, M.Z.; Bacova, P.; Bernabei, M.; Narros, A.; Likos, C.N.; Moreno, A.J.

ACS MACRO LETTERS 3, 611 (2014)

4

How far are single-chain polymer nanoparticles in solution from the globular state?

Pomposo, J.A.; Perez-Baena, I.; Lo Verso, F.; Moreno, A.J.; Arbe, A.; Colmenero, J.

ACS MACRO LETTERS 3, 767 (2014)

5

Metallo-folded single-chain nanoparticles with catalytic selectivity

Sanchez-Sanchez, A.; Arbe, A.; Colmenero, J.; Pomposo, J.A.

ACS MACRO LETTERS 3, 439 (2014)

6

Revealing the Adsorption Mechanisms of Nitroxides on Ultrapure, Metallicity-Sorted Carbon Nanotubes

Ruiz-Soria G; Paz AP; Sauer M; Mowbray DJ; Lacovig P; Dalmiglio M; Lizzit S; Yanagi K; Rubio A; Goldoni A; Ayala P; Pichler T.

ACS Nano 8, 1375 (2014)

7

Spectroscopic fingerprints of work-function-controlled phthalocyanine charging on metal surfaces

Borghetti, P.; El-Sayed, A.; Goiri, E.; Rogero, C.; Lobo-Checa, J.; Floreano, L.; Ortega, J.E.; De Oteyza, D.G.

ACS Nano 8, 12786 (2014)

8

Orbital Redistribution in Molecular Nanostructures Mediated by Metal-Organic Bonds

Yang ZC, Corso M, Robles R, Lotze C, Fitzner R, Mena-Osteritz E, Bauerle P, Franke KJ, Pascual JI.

ACS Nano 8, 10715 (2014)

9

Unoccupied electronic structure and relaxation dynamics of Pb/Si(111)

Sandhofer M, Sklyadneva IY, Sharma V, Trontl VM, Zhou P, Ligges M, Heid R, Bohnen KP, Chulkov EV, Bovensiepen U.

Journal of Electron Spectroscopy and Related Phenomena 195, 278 (2014)

10

Mechanically Interlocked Single-Wall Carbon Nanotubes

de Juan A; Pouillon Y; Ruiz-Gonzalez L; Torres-Pardo A; Casado S; Martin N; Rubio A; Perez EM.

Angewandte Chemie International Edition 53, 5394 (2014)

11

Lasing threshold of one- and two-photon-pumped dye-doped silica powder

García-Ramiro, B.; Illarramendi, M.A.; García-Revilla, S.; Balda, R.; Levy, D.; Zayat, M.; Fernández, J.

Applied Physics B: Lasers and Optics 117, 1135 (2014)

12

Photo-induced strengthening of weak bonding in noble gas dimers

Miyamoto Y; Miyazaki T; Rubio A; Zhang H.

Applied Physics Letters 104, 201107 (2014)

13

Proposal for a phase-coherent thermoelectric transistor

Giazotto F; Robinson JWA; Moodera JS; Bergeret FS.

Applied Physics Letters 105, 062602 (2014)

14

Proximity nanovalve with large phase-tunable thermal conductance

Strambini, E.; Bergeret, F.S.; Giazotto, F.

Applied Physics Letters 105, 082601 (2014)

15

PH-responsive single-chain polymer nanoparticles utilising dynamic covalent enamine bonds

Sanchez-Sanchez, A.; Fulton, D.A.; Pomposo, J.A.

Chemical Communications 50, 1871 (2014)

16

Adsorption of tetrathiafulvalene (TTF) on Cu(1 0 0): Can π-stacked 1-D aggregates be formed at low temperature?

Sarasola, A.; Barja, S.; Vázquez De Parga, A.L.; Arnau, A.

Chemical Physics Letters 612, 45 (2014)

17

Component dynamics in nanostructured PI-PDMS diblock copolymers with PI segregated in lamellas, cylinders, and spheres

Alegria A; Lund R; Barroso-Bujans F; Arbe A; Colmenero J.

Colloid and Polymer Science 292, 1863 (2014)

18

An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions

Mostofi AA; Yates JR; Pizzi G; Lee YS; Souza I; Vanderbilt D; Marzari N

Computer Physics Communications 185, 2309 (2014)

19

PFO-BPy solubilizers for SWNTs: Modelling of polymers from oligomers

Glanzmann LN, Mowbray DJ, Rubio A.

Physica Status Solidi B-Basic Solid State Physics 251, 2407 (2014)

20

Cross-Conjugation vs. Linear Conjugation in Donor-Bridge-Acceptor Nitrophenol Chromophores

Christensen MA; Della Pia EA; Houmoller J; Thomsen S; Wanko M; Bond AD; Rubio A; Nielsen SB; Nielsen MB.

European Journal of Organic Chemistry 2014, 2044 (2014)

21

High pressure phases of different tetraboranes

Suarez-Alcubilla, A.; Gurtubay, I.G.; Bergara, A.

High Pressure Research 34, 59 (2014)

22

Application of the level set method for the visual representation of continuous cellular automata oriented to anisotropic wet etching

Montolíu, C.; Ferrando, N.; Cerdá, J.; Colom Palero, R. J.

International Journal of Computer Mathematics 91, 124 (2014)

23

Hole-phonon relaxation and photocatalytic properties of titanium dioxide and zinc oxide: first-principles approach

Zhukov VP; Tyuterev VG; Chulkov EV; Echenique PM.

International Journal of Photoenergy 2014 (2014)

24

Are There Really Cooper Pairs and Persistent Currents in Aromatic Molecules?

Squire RH; March NH; Rubio A.

International Journal of Quantum Chemistry 114, 437 (2014)

25

Superconducting pairing mediated by spin fluctuations from first principles

Essenberger F, Sanna A, Linscheid A, Tandetzky F, Profeta G, Cudazzo P, Gross EKU.

Physical review B 90, 214504 (2014)

26

Atomic structure and phonons of a Pb ultrathin film on the Al(100) surface

Rusina, G.G.; Borisova, S.D.; Chulkov, E.V.

JETP Letters 100, 237 (2014)

27

Dynamics of the BiTeI lattice at high pressures

Ponosov, Y.S.; Kuznetsova, T.V.; Tereshchenko, O.E.; Kokh, K.A.; Chulkov, E.V.

JETP Letters 98, 557 (2014)

28

Engineering near-surface electron states in three-dimensional topological insulators

Men'shov, V.N.; Tugushev, V.V.; Chulkov, E.V.

JETP Letters 98, 603 (2014)

29

Dielectric spectroscopy at the nanoscale by atomic force microscopy: A simple model linking materials properties and experimental response

Miccio, L.A.; Kummali, M.M.; Schwartz, G.A.; Alegría, Á.; Colmenero, J.

Journal of Applied Physics 115, 184305 (2014)

30

Local versus global electronic properties of chalcopyrite alloys: X-ray absorption spectroscopy and ab initio calculations

Sarmiento-Perez R; Botti S; Schnohr CS; Lauermann I; Rubio A; Johnson B.

Journal of Applied Physics 116, 093703 (2014)

31

Ab initio molecular dynamics calculations on scattering of hyperthermal H atoms from Cu(111) and Au(111)

Kroes, G.-J.; Pavanello, M.; Blanco-Rey, M.; Alducin, M.; Auerbach, D.J.

Journal of Chemical Physics, 141, 054705 (2014)

32

Dielectric spectra broadening as a signature for dipole-matrix interaction. IV. Water in amino acids solutions

Levy, E.; Cerveny, S.; Ermolina, I.; Puzenko, A.; Feldman, Y.

Journal of Chemical Physics 140, 135104 (2014)

33

Quasi-particle energy spectra in local reduced density matrix functional theory

Lathiotakis NN; Helbig N; Rubio A; Gidopoulos NI.

Journal of Chemical Physics 141, 164120 (2014)

34

Vibrational lifetimes of hydrogen on lead films: An ab initio molecular dynamics with electronic friction (AIMDEF) study

Saalfrank, P.; Juaristi, J.I.; Alducin, M.; Blanco-Rey, M.; Muiño, R.D.

Journal of Chemical Physics 141, 234702 (2014)

35

Nonadiabatic and Time-Resolved Photoelectron Spectroscopy for Molecular Systems

Flick J; Appel H; Rubio A.

Journal of Chemical Theory and Computation 10, 1665 (2014)

36

Quasiparticle level alignment for photocatalytic interfaces

Migani, A.; Mowbray, D.J.; Zhao, J.; Petek, H.; Rubio, A.

Journal of Chemical Theory and Computation 10, 2103 (2014)

37

A survey of the parallel performance and accuracy of Poisson solvers for electronic structure calculations

García-Risueño, P.; Alberdi-Rodriguez, J.; Oliveira, M.J.T.; Andrade, X.; Pippig, M.; Muguerza, J.; Arruabarrena, A.; Rubio, A.

Journal of Computational Chemistry 35, 427 (2014)

38

Electron dynamics of unoccupied states in topological insulators

Niesner, D.; Otto, S.; Fauster, Th.; Chulkov, E.V.; Eremeev, S.V.; Tereshchenko, O.E.; Kokh, K.A.

Journal of Electron Spectroscopy and Related Phenomena 195, 258 (2014)

39

Image potential eigenstates and resonances on the (110) surfaces of noble metals: Energies and lifetimes

Tsirkin, S.S.; Chulkov, E.V.

Journal of Experimental and Theoretical Physics 118, 167 (2014)

40

Effect of Tm^{3+} codoping on the near-infrared and upconversion emissions of Er^{3+} in TeO_2-ZnO-ZnF_2 glasses

Miguel, A.; Arriandiaga, M.A.; Morea, R.; Fernandez, J.; Gonzalo, J.; Balda, R.

Journal of Luminescence 154, 136 (2014)

41

Whispering gallery mode emission from a composite system of J-aggregates and photonic microcavity

Melnikau, D.; Savateeva, D.; Rusakov, K.I.; Rakovich, Y.P.

Journal of Luminescence 145, 138 (2014)

42

Resistive switching dependence on atomic layer deposition parameters in HfO2-based memory devices

Zazpe, R.; Ungureanu, M.; Golmar, F.; Stoliar, P.; Llopis, R.; Casanova, F.; Pickup, D.F.; Rogero, C.; Hueso, L.E.

Journal of Materials Chemistry C 2, 3204 (2014)

43

Anisotropic etching on Si{1 1 0}: Experiment and simulation for the formation of microstructures with convex corners

Pal, P.; Gosalvez, M.A.; Sato, K.; Hida, H.; Xing, Y.

Journal of Micromechanics and Microengineering 24, 125001 (2014)

44

Linear and nonlinear optical effects induced by energy transfer from semiconductor nanoparticles to photosynthetic biological systems

Rakovich, A.; Donegan, J.F.; Oleinikov, V.; Molinari, M.; Sukhanova, A.; Nabiev, I.; Rakovich, Y.P.

Journal of Photochemistry and Photobiology C: Photochemistry Reviews 20, 17 (2014)

45

Antiferromagnetism in nanofilms of Mn-doped GaN

Echeverría-Arrondo, C.; Pérez-Conde, J.; Ayuela, A.

Journal of Physical Chemistry C 118, 18064 (2014)

46

Asymmetric response toward molecular fluorination in binary copper-phthalocyanine/pentacene assemblies

De Oteyza, D.G.; Garcia-Lastra, J.M.; Goiri, E.; El-Sayed, A.; Wakayama, Y.; Ortega, J.E.

Journal of Physical Chemistry C 118, 18626 (2014)

47

Evolutionary Kinetic Monte Carlo: Atomistic rates of surface-mediated processes from surface morphologies

Ferrando, N.; Gosalvez, M.A.; Ayuela, A.

Journal of Physical Chemistry C 118, 11636 (2014)

48

Exploring the surface chemical reactivity of single crystals of binary and ternary bismuth chalcogenides

Politano, A.; Caputo, M.; Nappini, S.; Bondino, F.; Magnano, E.; Aliev, Z.S.; Babanly, M.B.; Goldoni, A.; Chiarello, G.; Chulkov, E.V.

Journal of Physical Chemistry C 118, 21517 (2014)

49

Forster-Induced Energy Transfer in Functionalized Graphene

Malic E; Appel H; Hofmann OT; Rubio A.

Journal of Physical Chemistry C 118, 9283 (2014)

50

Identifying highly conducting Au-C links through inelastic electron tunneling spectroscopy

Foti, G.; Vázquez, H.; Sánchez-Portal, D.; Arnau, A.; Frederiksen, T.

Journal of Physical Chemistry C 118, 27106 (2014)

51

Massive surface reshaping mediated by metal-organic complexes

Abadía, M.; González-Moreno, R.; Sarasola, A.; Otero-Irurueta, G.; Verdini, A.; Floreano, L.; Garcia-Lekue, A.; Rogero, C.

Journal of Physical Chemistry C 118, 29704 (2014)

52

Modeling ferro- and antiferromagnetic interactions in metal-organic coordination networks

Faraggi, M.N.; Golovach, V.N.; Stepanow, S.; Tseng, T.-C.; Abdurakhmanova, N.; Kley, C.S.; Langner, A.; Sessi, V.; Kern, K.; Arnau, A.

Journal of Physical Chemistry C 119, 547 (2014)

53

Resonant lifetime of core-excited organic adsorbates from first principles

Fratesi, G.; Motta, C.; Trioni, M.I.; Brivio, G.P.; Sánchez-Portal, D.

Journal of Physical Chemistry C 118, 8775 (2014)

54

Size distribution and frustrated antiferromagnetic coupling effects on the magnetic behavior of ultrafine akaganéite (β-FeOOH) Nanoparticles

Luna, C.; Ilyn, M.; Vega, V.; Prida, V.M.; González, J.; Mendoza-Reséndez, R.

Journal of Physical Chemistry C 118, 21128 (2014)

55

Modelling the effect of nuclear motion on the attosecond time-resolved photoelectron spectra of ethylene

Crawford-Uranga A; De Giovannini U; Mowbray DJ; Kurth S; Rubio A.

Journal of Physics B: Atomic, Molecular and Optical Physics 47, 124018 (2014)

56

Dynamics and thermodynamics of polymer glasses

Cangialosi D.

Journal of Physics Condensed Matter 26, 153101 (2014)

57

Modelling near-surface bound electron states in a 3D topological insulator: analytical and numerical approaches

Men'shov VN; Tugushev VV; Menshchikova TV; Eremeev SV; Echenique PM; Chulkov EV

Journal of Physics Condensed Matter 26, 485003 (2014)

58

Relaxation of highly excited carriers in wide-gap semiconductors

Tyuterev VG; Zhukov VP; Echenique PM; Chulkov EV.

Journal of Physics Condensed Matter 27, 025801 (2014)

59

Structural modifications of gold thin films produced by thiol-derivatized single-stranded DNA immobilization

Arroyo-Hernández, M.; Svec, M.; Rogero, C.; Briones, C.; Martín-Gago, J.Á.; Costa-Krämer, J.L.

Journal of Physics Condensed Matter 26, 055010 (2014)

60

Quantum Spin Hall Effect in Two-Dimensional Crystals of Transition-Metal Dichalcogenides

Cazalilla MA, Ochoa H, Guinea F.

Physical review Letters 113, 077201 (2014)

61

Electron-phonon coupling in quantum-well states of the Pb/Si(1 1 1) system

Ligges, M.; Sandhofer, M.; Sklyadneva, I.; Heid, R.; Bohnen, K.-P.; Freutel, S.; Rettig, L.; Zhou, P.; Echenique, P.M.; Chulkov, E.V.; Bovensiepen, U.

Journal of physics. Condensed matter : an Institute of Physics journal 26, 352001 (2014)

62

Structural characterization of slightly boron-deficient LiB, $LiB_{0.9}$ and $LiB_{0.8}$, under pressure

Suarez-Alcubilla, A.; Gurtubay, I.G.; Bergara, A.

Journal of physics. Condensed matter : an Institute of Physics journal 26, 475402 (2014)

63

Single-chain nanoparticles vs. star, hyperbranched and dendrimeric polymers: Effect of the nanoscopic architecture on the flow properties of diluted solutions

Perez-Baena, I.; Moreno, A.J.; Colmenero, J.; Pomposo, J.A.

Soft Matter 10, 9454 (2014)

64

Coulomb edge effects in graphene nanoribbons

Jaskolski, W.; Ayuela, A.

Solid State Communications 196, 1 (2014)

65

Multiple scattering calculations for nonreciprocal planar magnetoplasmonic nanostructures

Christofi, A.; Tserkezis, C.; Stefanou, N.

Journal of Quantitative Spectroscopy and Radiative Transfer 146, 34 (2014)

66

Photoinduced C-C Reactions on Insulators toward Photolithography of Graphene Nanoarchitectures

Palma CA; Diller K; Berger R; Welle A; Bjork J; Cabellos JL; Mowbray DJ; Papageorgiou AC; Ivleva NP; Matich S; Margapoti E; Niessner R; Menges B; Reichert J; Feng XL; Rader HJ; Klappenberger F; Rubio A; Mullen K; Barth JV.

Journal of the American Chemical Society 136, 4651 (2014)

67

Structural, optical, and spectroscopic properties of Er^{3+}-doped TeO_2-ZnO-ZnF_2 glass-ceramics

Miguel, A.; Morea, R.; Arriandiaga, M.A.; Hernandez, M.; Ferrer, F.J.; Domingo, C.; Fernandez-Navarro, J.M.; Gonzalo, J.; Fernandez, J.; Balda, R.

Journal of the European Ceramic Society 34, 3959 (2014)

68

Time-resolved random laser spectroscopy of inhomogeneously broadened systems

Fernández, J.; García-Revilla, S.; Carlos, L.D.; Pecoraro, E.; Arriandiaga, M.A.; Balda, R.

Laser and Photonics Reviews, 8, L32 (2014)

69

Branch-point motion in architecturally complex polymers: Estimation of hopping parameters from computer simulations and experiments

Bacová, P.; Lentzakis, H.; Read, D.J.; Moreno, A.J.; Vlassopoulos, D.; Das, C.

Macromolecules 47, 3362 (2014)

70

Collective features in polyisobutylene. A study of the static and dynamic structure factor by molecular dynamics simulations

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

Macromolecules 47, 447 (2014)

71

Efficient route to compact single-chain nanoparticles: Photoactivated synthesis via thiol-yne coupling reaction

Perez-Baena, I.; Asenjo-Sanz, I.; Arbe, A.; Moreno, A.J.; Lo Verso, F.; Colmenero, J.; Pomposo, J.A.

Macromolecules 47, 8270 (2014)

72

Intercalation and confinement of poly(ethylene oxide) in porous carbon nanoparticles with controlled morphologies

Barroso-Bujans, F.; Palomino, P.; Fernandez-Alonso, F.; Rudić, S.; Alegría, A.; Colmenero, J.; Enciso, E.

Macromolecules 47, 8729 (2014)

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BOOK CHAPTERS

- **Equilibrium and Out-of-Equilibrium Dynamics in Confined Polymers and Other Glass Forming Systems by Dielectric Spectroscopy and Calorimetric Techniques**

  By Cangialosi, D

  Dynamics in geometrical Confinement

  Edited By Friedrich Kremer

  Pages 339-361 Published 2014

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- **Gas Sensing and Thermal Transport Through Carbon-Nanotube-Based Nanodevices**

  By: Pouillon, Y.; Perez Paz, A.; Maklin, J.; Halonen, N.; Leroy, Y. ; Mowbray, D.; Garcia Lastra, J. M; Toth, G. ; Kordas, K. ; Konya, Z.; Kukovecz, A.; Rubio, A.

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Conferences

CFM scientists have organized or coorganized 7 workshops and conferences in the year 2014. Most of these meetings have been held in close cooperation with Donostia Intenational Physics Center (DIPC), which proves the excellent results brought by the synergy between both institutions. The list follows:

- **Photoluminescence in rare earths (PRE´14): Photonic materials and devices**
  May 14-16, 2014. Donostia / San Sebastián - Joaquin Fernandez (CFM) and Rolindes Balda (CFM)

- **Trends in (Nano)Photonics 2014**
  July 24-24, 2014. Donostia / San Sebastián - Javier Aizpurua (CFM)

- **Light in a hole: Workshop on confining light and molecules**
  August 18-19, 2014. Donostia / San Sebastián - Javier Aizpurua (CFM)

- **Fuerzas y Túnel 2014**
  August 27-29, 2014. Donostia / San Sebastián - Celia Rogero Blanco (CFM), Fernando Moreno (CSIC)

- **3th Baskrete - Industry open days**
  September 16-17, 2014. Donostia / San Sebastián - CEI Euskampus - EHU/UPV - DIPC - Tecnalia - CFM - CIC nanoGUNE - Andres Ayuela (CFM), Jorge Sanchez-Dolado (TECNALIA)

- **GDRi 2014**
  September 28 - Octubre 1, 2014. Donostia / San Sebastián - Roland Pellenq (MIT, CNRS), Emanuela Delgado (ETH Zurich), Pierre Levitz (CNRS), Jorge Sanchez-Dolado (TECNALIA), Andres Ayuela (CFM)

- **Razón, Intuición e Imaginación en Ciencia y en Literatura**
  November 18-19, 2014. Donostia / San Sebastián - Gustavo Ariel Schwartz (CFM)

Research Funding

The list of funding grants obtained by CFM scientists that were active during the year 2014 follows:

FIS2010-19609-C02-02
Propiedades electrónicas y reactividad de sistemas complejos
PI: Díez Muiño

FIS2010-19609-C02-01
Dinámica electrónica, transporte, plasmónica y microscopía electrónica
PI: A. Arnau

FIS2011-28851-C02-02
Propiedades de transporte electrónico en nanoestructuras híbridas: superconductores, ferromagnetos y metales normales.
PI: Sebastian Bergeret

IE11-304 nanoIKER'11
NanoIKER'11-I+D en Nanociencia y Nanotecnología: Magnetismo, Polímeros, Fotónica, Cementos y Grafeno.

Grant Agreement 267374, 7PM-IDEAS
DYNAMO- Dynamical processes in open quantum systems: pushing the frontiers of theoretical spectroscopy.
PI: A. Rubio

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. Fernandez

IT654-13
Grupos de Investigación Consolidados / de Alto Rendimiento: "Polímeros y materiales no cristalinos"
PI: Juan Colmenero de León

IT578-13
Grupos de Investigación Consolidados / de Alto Rendimiento: "Energy Materials: Fundamental developments in ab-initio computational Material Science"
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: Daniel Sanchez Portal

MAT2012-33720
Efectos magnetoeléctricos estáticos y ópticos en cristales
PI: I. Souza

PITN-GA-2012-316633
Polymer - Carbon Nanotubes Active Systems for Photovoltaics POCAONTAS
PI: A. Rubio

NMP3-SL-2012-28087
Time dynamics and Control in naNOStructures for magnetic recording and energy applications
P.I: A. Rubio

FIS2013-41184-P
Optoelectrónica de gaps (sub)nanométricos plasmónicos para el desarrollo de espectroscopías y microscopías aumentadas por campo
PI: Aizpurua Iriazabal,Francisco Javier

MAT2013-46593-C6-2-P
Teoría de propiedades electrónicas de híbridos covalentes en superficies
PI: Sanchez Portal,Daniel

FIS2013-48286-C2-1-P
Electronic processes in surfaces and nanostructures
PI: Ayuela Fernandez, Andres

FIS2013-48286-C2-2-P
Reactividad, propiedades electrónicas y estructurales de sistemas complejos
PI: Juaristi Oliden, Joseba Iñaki

2014-CIEN-000135-01
Sistemas Sostenibles: Manipulador criogénico de He de circuito cerrado
PI: E. Ortega

IT659-13
Grupo de Investigación Consolidado
PI: Rolindes Balda

MAT2013-48246-C2-2-P
Efecto del procesamiento sobre las propiedades ópticas de vidrios y vitrocerámicos con aplicaciones fotónicas
PI: Rolindes Balda

S-PE12UN016
Desarrollo de vitrocerámicos eutécticos biocompatibles dopados con tierras raras para aplicaciones en dispositivos fotónicos
PI: Rolindes Balda

PIB2010US-00652
International Collaboration in Chemistry: Molecules at Nanostructured Surfaces for Solar Cell Applications.
IP: J. Enrique Ortega

MAT2013-46593-C6-4P
Hibridos covalentes en superficies
PI: J. Enrique Ortega

7PM – People- CIG13/02
Magnetoelectric couplings in solids and releated phenomena
PI: I. Souza

PIEF-GA-2013-622934
Optchatra
PI: A. Rubio

FP7 – PEOPLE – 2013 –IEF
PHOTOPROTEIN – Photophysics of Fluorescent Proteins
PI: A. Rubio

PIIF- GA -2012 – 326435
RespSpatDisp
PI: A. Rubio

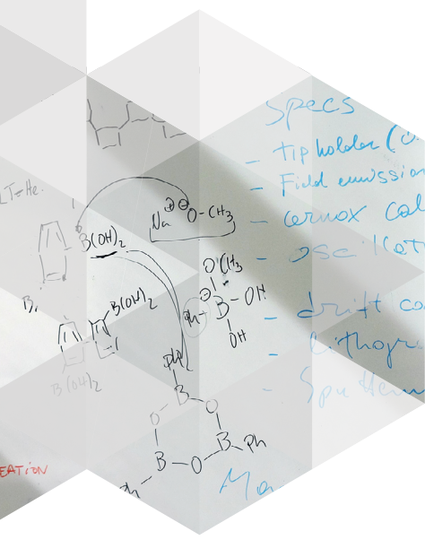
FIS201346159-C3-1-P
Desarrollos fundamentales para la simulación y caracterización de procesos dinámicos fuera del equilibrio en sistemas moleculares "energy materials" (FUN-EMAT)
PI: A. Rubio

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

IT627-13
Grupo de Investigación Consolidado.
IP Lucia Vitali

PRO-MAG2D/S – PE12UN095
Propiedades magnéticas y electrónicas de aleaciones bidimensionales de gadolinio con moléculas orgánicas.
IP. Lucia Vitali

MAT2013-46593-C6-4-P
Híbridos covalentes en superficies
PI: Enrique Ortega / Lucia Vitali



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/MPC 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 2014 follows:

PhD Theses

1.
Structure and Electronics of Donor-Acceptor Blends
Elizabeth Goiri Little
2014/02/28
Supervisor: Dimas G. de Oteyza y J. Enrique Ortega
UPV/EHU

2.
Transport phenomena in superconducting hybrid nanostructures
Asier Ozaeta
2014/09/05
Supervisor: Sebastian Bergeret
UPV/EHU

3.
Computational investigation of chain dynamics in architecturally complex polymers
Petra Bacova
2014/07/07
Supervisor: Angel Moreno
UPV/EHU

4.
Assembly & disassembly of bioinspired single-chain polymer nanoparticles
Ana Belén Sánchez Sánchez
2014/12/15
Supervisor: José A. Pomposo
UPV/EHU

5.
From polymer chains to enzyme-mimetic soft nanoparticles
Irma Perez Baena
2014/11/24
Supervisor: José A. Pomposo
UPV/EHU

6.
Elastic and inelastic electron transport through alkane-based molecular junctions
Giuseppe Foti
2014
Supervisor: Thomas Frederiksen
UPV/EHU

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

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, sharing efforts with DIPC. The list of visiting schools follows:

		SCHOOL/GROUP	Nº
07/03/2014	Larramendi ikastetxea	4º ESO	32
30/04/2014	Presentación de María ikastetxea	4º ESO	25
21/03/2014	IES Leizaran, Andoain	1º y 2º Bachiller	30
30/05/2014	IPINTZA Bergarako Institutua	1º Bachiller	13
04/04/2014	Beasain BHI	2º Bachiller	28
11/04/2014	Usandizaga Institutua	2º Bachiller	41
16/05/2014	Urretxu Zumarraga Ikastola	2º Bachiller	29

Other outreach activities:

- **Semana de la Ciencia - Donostia-San Sebastian** 6-8/11/2014
- **Promoción aulas de la Experiencia - Pamplona** 12/12/2014

Knowledge Transfer

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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